

ANUÁRIO CIENTÍFICO 2007

Resumos de Artigos, Comunicações, Teses e Livros



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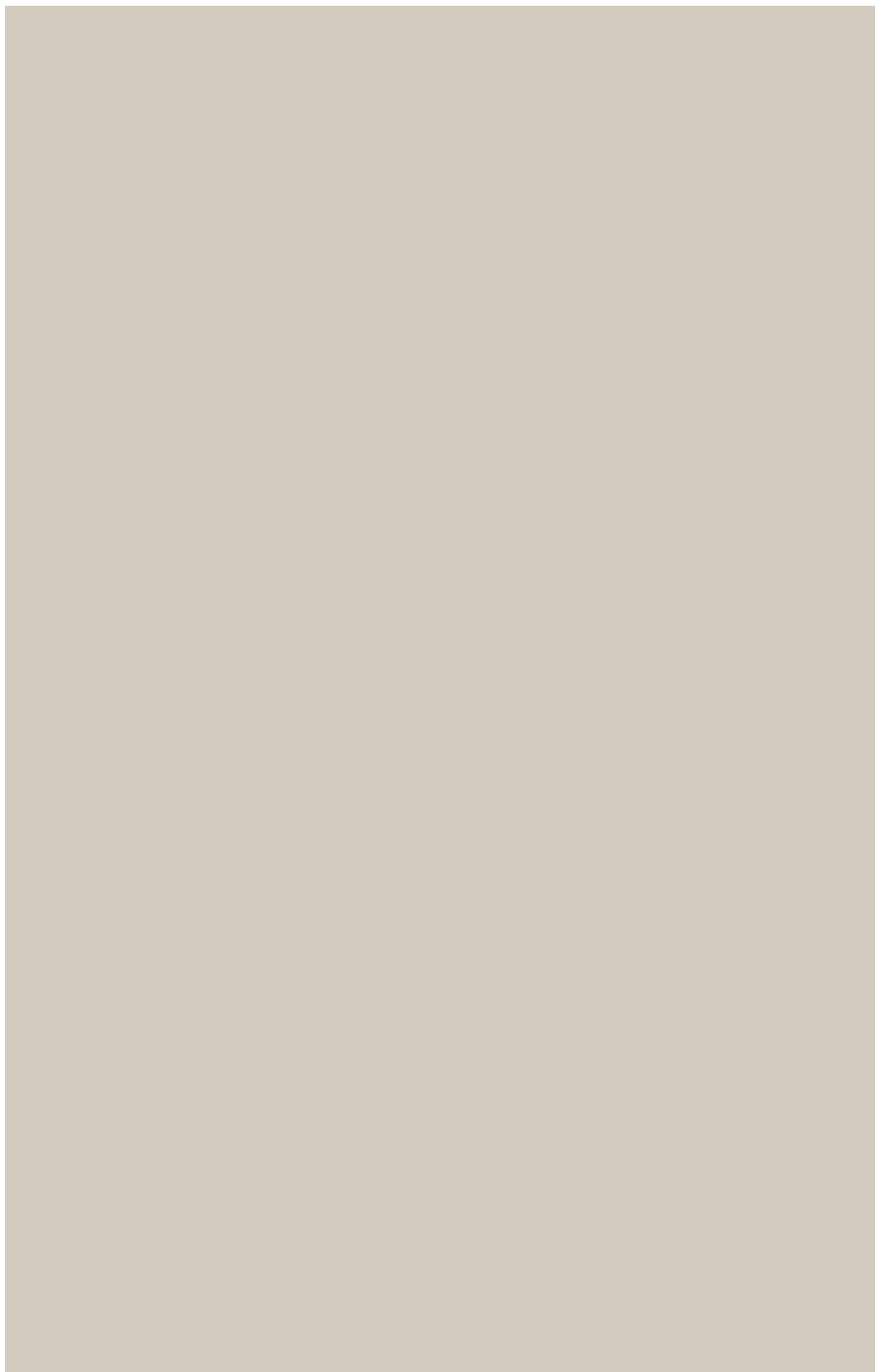
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O Presidente do Conselho Científico



(Prof. José A. Paixão Coelho)



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- 03** ENGENHARIA MECÂNICA
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01

ENGENHARIA CIVIL

Anuário Científico 2007

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SISTEMAS DE IMPERMEABILIZAÇÃO E DRENAGEM DE TÚNEIS EM ESCAVAÇÃO. MATERIAIS CONSTITUINTES E SUA COLOCAÇÃO

Justo, J.¹; Lopes, M.G.²; Brito, J.³

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Muito embora a construção de obras subterrâneas seja muito antiga, a preocupação efectiva com a sua impermeabilização é bastante mais recente. Em Portugal, só há cerca de uma década é que grande parte dos túneis em escavação é contemplado com um sistema de impermeabilização contínuo. Tendo em consideração que os conhecimentos sobre estes sistemas têm sido pouco divulgados, julgou-se oportuno neste artigo descrever os materiais constituintes destes sistemas. E chamar a atenção para algumas particularidades da sua colocação.

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Revista Engenharia e Vida nº 34, Abril de 2007.

SISTEMAS DE IMPERMEABILIZAÇÃO E DRENAGEM DE TÚNEIS EM ESCAVAÇÃO. INSTALAÇÃO E CONTROLO DE QUALIDADE

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Civil nº 29, Setembro
de 2007.*

Nas obras subterrâneas, a preocupação efectiva com a sua impermeabilização é ainda recente. Nestas obras as anomalias dos sistemas de impermeabilização e drenagem associada são, regra geral, difíceis de solucionar, sendo normalmente onerosas e por vezes pouco fiáveis. Assim, é imprescindível, para assegurar a funcionalidade e durabilidade desses sistemas, a existência de um controlo rigoroso das actividades relativas à instalação dos materiais que o constituem. Neste artigo são descritas as actividades de controlo indispensáveis à garantia da qualidade do sistema de impermeabilização e drenagem associada, chamando-se a atenção para a sua necessidade.

GUIDELINES FOR GOOD PRACTICE OF WATER REUSE FOR IRRIGATION: PORTUGUESE STANDARD NP 4434

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The growing number of municipal wastewater treatment plants in Portugal delivers about 500 million m³ of treated wastewater that is discharged in river and coastal waters, still representing a pollutant load to receiving waters and yet the waste of water resources which could be successfully used for agricultural and landscape irrigation, golf courses, water reservoirs for fire protection. Because water reuse can contribute to the economic development it must be stimulated by central, regional and local authorities, but within the framework of good practices and their monitoring. This chapter presents the new Portuguese standard NP 4434 that presents guidelines on water quality, irrigation practice, management of environmental impacts, protection of public and animal health and aspects of control and monitoring.

Publicado em:

Zaidi, M.K. (Ed.) - *Wastewater Reuse - Risk Assessment, Decision-Making and Environmental Security*, Amsterdam, Springer, pp. 253-265, 2007.

THE SOURCE OF THE 1722 ALGARVE EARTHQUAKE: EVIDENCE FROM MCS AND TSUNAMI DATA

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The 27 December 1722 Algarve earthquake destroyed a large area in southern Portugal generating a local tsunami that inundated the shallow areas of Tavira. It is unclear whether its source was located onshore or offshore and, in any case, what was the tectonic source responsible for the event. We analyze available historical information concerning macroseismicity and the tsunami to discuss the most probable location of the source. We also review available seismotectonic knowledge of the offshore region close to the probable epicenter, selecting a set of four candidate sources. We simulate tsunamis produced by these candidate sources assuming that the sea bottom displacement is caused by a compressive dislocation over a rectangular fault, as given by the half-space homogeneous elastic approach, and we use numerical modeling to study wave propagation and run-up. We conclude that the 27 December 1722 Tavira earthquake and tsunami was probably generated offshore, close to 37°01'N, 7°49'W.

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*Journal of
Seismology*, 2007,
11:371-380 doi
10.1007/s10950-007-
9058-y.

CHLORINATION OF 2-PHENOXYPROPANOIC ACID WITH NCP IN AQUEOUS ACETIC ACID: USING A NOVEL ORTHO-PARA RELATIONSHIP AND THE PARA/META RATIO OF SUBSTITUENT EFFECTS FOR MECHANISM ELUCIDATION

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Rate constants were measured for the oxidative chlorodehydrogenation of (*R,S*)-2-phenoxypropanoic acid and nine *ortho*-, ten *para*- and five *meta*-substituted derivatives using (*R,S*)-1-chloro-3-methyl-2,6-diphenylpiperidin-4-one (NCP) as chlorinating agent. The kinetics was run in 50% (v/v) aqueous acetic acid acidified with perchloric acid under pseudo-first order conditions with respect to NCP at temperature intervals of 5K between 298K and 318K, except at the highest temperature for the *meta* derivatives. The dependence of rate constants on temperature was analysed in terms of the isokinetic relationship (IKR). For the 20 reactions studied at 5 different temperatures, the isokinetic temperature was estimated to be 382K, which suggests the preferential involvement of water molecules in the rate-determining step. The dependence of rate constants on *meta* and *para* substitution was analysed using the tetralinear extension of the Hammett equation. The parameter λ for the *para/meta* ratio of polar substituent effects was estimated to be 0.926 and its electrostatic modelling suggests the formation of an activated complex bearing an electric charge near the oxygen atom belonging to the phenoxy group. A new approach is introduced for examining the effect of *ortho* substituents on reaction rates. Using IKR-determined values of activation enthalpies for a set of nine pairs of substrates with a given substituent, a linear correlation is found between activation enthalpies of *ortho* and *para* derivatives. The correlation is interpreted in terms of the selectivity of the reactant towards *para*- or *ortho*-monosubstituted substrates, the slope of which being related to the *ortho* effect. This slope is thought to be approximated by the ratio of polar substituent effects from *ortho* and *para* positions in benzene derivatives. Using the electrostatic theory of through-space interactions and a dipole length of 0.153nm, this ratio was calculated at various positions of a charged reaction centre along the benzene C₁-C₄ axis, being about 2.5 near the ring and decreasing steeply with increasing distance until reaching a minimum value of -0.565 at 1.3nm beyond the aromatic ring. Activation enthalpies and entropies were estimated for substrates bearing the isoselective substituent in either *ortho* and *para*

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positions, being demonstrated that they are much different from the values for the parent substrate. The electrophilic attack on the phenolic oxygen atom by the protonated chlorinating agent is proposed as the rate-determining step, this step being followed by the fast rearrangement of the intermediate thus formed, leading to products containing chlorine in the aromatic ring.

GYPSUM COATINGS IN ANCIENT BUILDINGS

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Gypsum plasters from old buildings are a legacy of the building techniques of our ancestors. These coatings, frequently gifted with a high artistic value, are part of the historical building heritage of each country that needs to be well known and preserved.

The present paper begins with a general overview of the history of gypsum plasters in Portugal, since the most ancient traces in the Roman period until modern plasters.

A description of the main coats that constitute traditional gypsum plasters follows: the lime mortar undercoat, the lime, gypsum and sand preparation coat with a thickness of 3-5mm and the gypsum finishing coat, made of gypsum and air lime slurry.

Next, the constitution of the backgrounds is described, namely of the timber main walls and the partition wall typical of the anti-seismic *Pombalina* construction used in Lisbon after the 1755 earthquake. Finally, the constitutions of the several plaster coats and their production and application process are referred to.

Publicado em:

*Construction and
Building Materials,
Volume 21, Issue 1,
January 2007, 126-131.*

FORECASTING ERRORS IN CAPITAL BUDGETING: A MULTI-FIRM POST-AUDIT

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Economist*, 2007, 52-1,
21-39.

This is a post-audit study concerning the accuracy of capital budgeting procedures. It is based on the statistical analysis of the deviations occurring between effective and forecasted performance of companies after implementing their projected investments. The forecasts were collected from a large database of applications for investment incentives submitted for consideration to the Portuguese Governmental Agency IAPMEI during the 2nd European Union Framework Programme. The first conclusion of the study is the significance of negative forecasting errors of post-investment sales and their implication in terms of the expected profitability. In contrast, forecasts on future operating costs were quite accurate and errors on investment expenses revealed high volatility. Also interesting is the finding that there seems to be no relationship between the size, industry, region or investment incentives and the pattern of the errors found.

MECHANICAL BEHAVIOUR OF CONCRETE MADE WITH FINE RECYCLED CONCRETE AGGREGATES

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This paper concerns the use of fine recycled concrete aggregates to partially or globally replace natural fine aggregates (sand) in the production of structural concrete. To evaluate the viability of this process, an experimental campaign was implemented in order to monitor the mechanical behaviour of such concrete. The results of the following tests are reported: compressive strength, split tensile strength, modulus of elasticity and abrasion resistance. From these results, it is reasonable to assume that the use of fine recycled concrete aggregates does not jeopardize the mechanical properties of concrete, for replacement ratios up to 30%.

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Cement and Concrete Composites, 2007, 29, 397-401.

WATER REUSE IN EUROPE

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Renewable water resources in Europe change widely from northern Atlantic to Mediterranean Sea as a direct consequence of climate (rainfall and temperature). The demand for water resources in Europe increased 600% during the second half of the 20th century. About 75% of abstracted fresh water in the EU for all uses comes from surface water, about 25% from groundwater and only minor contributions from reuse of treated wastewater and desalination of seawater. Abstractions rates must be sustainable in order to ensure the management and protection of water resources and related ecosystems. The sustainable use of national water resources implies that the annually abstracted water should not exceed a certain ratio of the renewable water resources. The future situation of sustainable water resources will depend basically on the trends of renovation of water resources (that will be affected by climate change and by pollution) and pressure for water abstraction (depending mainly on the evolution of sectoral water uses, population and urbanization growth, tourism, industry).

This paper presents a brief description of the situation in European countries concerning the water availability and water demand. The conclusion is that in most of the European continent the amount of water available largely exceeds water demand. However, severe imbalances between regions are observed: 4 countries in southern Europe (Cyprus, Italy, Malta and Spain) representing 18% of the European population are water stressed; 9 countries lying mainly in southern Europe, which represent 32% of European population, are moderately water stressed (Belgium, England, Germany, Check Republic, Bulgaria, Denmark, Portugal, Romania, Turkey).

Climate change is expected to reduce water availability and increase abstraction for irrigation in Mediterranean regions and Portugal. Under mid-range assumptions on temperature and precipitation changes, water availability is expected to decline in southern and southeastern Europe by 10% or more in some river basins.

The sectoral profile of water abstraction is expected to change in the long term: abstraction for power production is expected to decrease,

industrial water use is expected to stabilize or even to decline, urban water supply may increase significantly in eastern European countries and agriculture is expected to remain the largest water user mainly in the southern countries with the expected warmer and drier seasons resulting from climate change.

Water conservation is the hydrological answer to the problem of water imbalances. Water reuse is a very important strategic driving force for water conservation. Water can be reused for one or more beneficial purposes: agriculture and landscape irrigation, non-potable urban applications, groundwater recharge, recreational purposes and direct or indirect water supply.

Water reuse can have two important benefits. The most obvious is the provision of an alternative water resource. The second is the reduction of environmental impacts by reducing or eliminating wastewater disposal, which results in the preservation of water quality downstream. The path for water reuse will certainly be followed by many regions in Europe. European guidelines to assist the sustainability of water reuse are necessary.

ENVIRONMENTAL LIFE CYCLE ASSESSMENT (LCA) OF CONCRETE MADE WITH FINE RECYCLED CONCRETE AGGREGATES

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 Conference on
 Sustainable
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 12 a 14 de Setembro
 de 2007, pp. 789-794.*

The majority of worldwide structures use concrete as its main material. This happens because concrete is economically feasible, due to its undemanding production technology and ease of use.

However, it is widely recognized that concrete production has a strong environmental impact in the planet. Natural aggregates use is one of the most important problems of concrete production nowadays, since they are obtained from limited, and in some countries scarce, resources. In Portugal, although there are enough stone quarries to cover coarse aggregates needs for several more years, supplies of fine aggregates are becoming scarcer, especially in the northern part of the country.

On the other hand, as concrete structures' life cycle comes to an end, an urgent need emerges to establish technically and economically viable solutions for demolition debris, other than for use as road base and quarry fill.

This paper presents a partial life cycle assessment (LCA) of concrete made with fine recycled concrete aggregates performed with EcoConcrete tool. EcoConcrete is a tailor-made, interactive, learning and communications tool promoted by the Joint Project Group (JPG) on the LCA of concrete, to qualify and quantify the overall environment impact of concrete products. It consists of an interactive Excel-spreadsheet in which several environmental inputs (material quantities, distances from origin to production site, production processes) and outputs (material, energy, emissions to air, water, soil or waste) are collected in a life cycle inventory, and are then processed to determine the environmental impact (assessment) of the analyzed concrete, in terms of ozone layer depletion, smog or "greenhouse" effect.

INSIGHTS ON THE DEEP STRUCTURE OF THE IBERIA ABYSSAL PLAIN AND GALICIA BANK SOUTHERN EDGE FROM NEW MCS AND WIDE ANGLE DATA

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In the scope of the Portuguese Continental Shelf Extension Program, 1600km of 2D MCS reflection lines were acquired over the Iberia Abyssal Plain and the southern edge of the Galicia Bank. The survey ties in with other academic and industry surveys. It comprised four E-W lines, crossing from continental to oceanic crust along the Zone of Exhumed Continental Mantle, and two N-S lines crossing the Iberia abyssal plain from the Galicia Bank to the Tore seamount and the Tagus Abyssal plain. Additionally nine OBSs were deployed along the MCS IBo2 profile (roughly at 41°N). The MCS acquisition layout consisted in a streamer 8km long and an array of bolt long-life air guns (5720 cu.in.). In order to record deep reflections the record length was set to 18s. The E-W lines were Kirchoff pre-stack time (PSTM) and depth migrated (PSDM). Velocity model for the depth migration was obtained on the sedimentary cover by using a grid based tomography algorithm from Paradigm's Geodepth software, and constrained, from the basement to deeper sections, using IBo2 wide angle results and other published refraction studies on the area. Results show a clear improvement of the PSDM lines with respect to the original time migrated lines, especially in the deeper sections. A good agreement is verified between the wide-angle IBo2 velocity model and the coincident depth migrated MCS line. The basement topography is highly variable across the studied lines and suggests that the tectonic segmentation pattern of the margin is complex in this sector. Mid to High amplitude intra-basement reflectors are often observed: i) forming wedges internally defined by sets of sub-parallel reflectors, sometimes disrupted by high angle faults (pre-rift sequences?); ii) Consisting on several low angle intra-basement reflectors, interpretable as detachments faults, dipping both westward and eastward and reaching, in some cases, at least a depth of 20km. We discuss the implications of our interpretations, from these enhanced PSDM images, to the existing tectonic models for this segment of the West Iberian Margin.

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Eos Trans. AGU, 88(52), Fall Meet. Suppl., Abstract T41A-0366.

PRELIMINARY RESULTS FROM NEW WIDE-ANGLE AND MCS DATA AT SEISMIC LINE IBo2: THE SOUTHERN EDGE OF THE GALICIA BANK

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New seismic data at the southern edge of the Galicia Bank was acquired during the summer of 2006, in the scope of the Portuguese Continental Shelf Extension Program. In order to control the velocity structure of sedimentary infill and access the deep basement structure 9 OBSs were deployed along the MCS IBo2 profile. Shooting interval was 200 m. This profile crosses from thinned continental crust at the southern Galicia Interior Basin into the Iberia Abyssal Plain Ocean Continent Transition at $\sim 41^{\circ}\text{N}$, commonly interpreted as the Zone of Exhumed Continental Mantle.

The 6 OBSs recovered have been relocated by direct water arrival fit. First arrival 2D tomography of sedimentary and basement arrivals have been performed. The obtained velocities were used to constrain depth migration of the deeper structure coincident MCS line.

A median filter processing was applied to the wide-angle data in order to enhance near offset arrivals. These correlate well to the TWT sedimentary record of MCS data. Arrival time fit and amplitude modelling provided a 2D velocity model. The TWT of the sedimentary interfaces and the top of basement were used to control the layer topography. Preliminary results indicate a good agreement between the wide-angle velocity model and the coincident depth migrated MCS line.

SMALL TO LARGE SCALE HETEROGENEITY AND POTENTIAL FIELD SIGNATURE AT THE OCEAN-CONTINENT TRANSITION: SOUTH SEGMENT OF THE WEST IBERIAN MARGIN

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The crustal and lithospheric mantle structure was investigated along a 370km profile at the south segment of the west Iberian margin, from 12.9°W to 8.7°W, at approximately 38°N. The profile crosses from inland unthinned continental to oceanic crust, IAM5. Both MCS data and wide-angle, WA, data were considered. WA data set includes 6 OBSs and 2 inland seismic stations. Free air and total field magnetic anomalies profiles were extracted from available grided data.

WA data cinematic and dynamic modeling provided a 2D velocity model that proved to be consistent with the free air anomaly profile. Strong WA recorded diffractions were identified and modeled. 2.5D generalized inversion on pseudo-susceptibility was performed. A Bouguer gravity anomaly grid was calculated and a similar procedure was performed for the geoid. First and second derivatives grids of this surface and its upward continued surfaces were calculated to locate lineated lows and highs.

All considered data sets and modeling results indicate four main crustal domains: oceanic, transitional, thinning and continental. Within the transitional domain the WA and MCS data sets clearly suggests that the crust is very heterogeneous. A 70-80km long crustal complex structure is found to vary both horizontally and vertically. At the easternmost segment of the transitional domain the rapidly seaward thinning middle continental crust rests over a seaward thickening lower transitional crust. Strong WA diffractions were modeled to originate at this interface level. PmP phases are required to originate at this segment of the transitional domain favoring a predominant gabbroic composition for this lower transitional crust. The 12km thick exhumed continental crust at the eastern limit of the transitional domain vanishes 40km to the west, at the foot of the continental slope.

The OCT locates at the western segment of the transitional domain, having ~30-40km width. Here the crust is highly reflective at all levels, probably due to intrusive bodies. This low scale heterogeneity is also patent in the WA data and the modeled WA diffractors correlates well to intrusive bodies. Both magnetic and free air profiles modeling

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are also consistent to a major rock property contrast at this location, where high apparent susceptibility and density blocks were modeled. The Moho does not continuously show at the MCS data and a few of these dipping reflectors reach mantle depths. This eastern 30-40km segment of the TAP is a mass excess segment, bordered to the west by a set of margin parallel positive magnetic anomalies.

Significant differences are found when we compare this segment to the central and north segments of the west Iberia OCT. In the central and northern segments of the west Iberian margin the density contrast between thinned continental crust and the transitional crust (ZECM) clearly correlates to a ridge in the Bouguer corrected geoid surface. No similar feature is found at the southern segment of the west Iberian margin, where such large body of exhumed mantle at the OCT is hardly supported by the data. The south segment of the OCT has a clear margin parallel magnetic signature, not referred to occur at the central and north segments. The width of the OCT at the south segment is ~30-40km while at the central segment is more than 150km. Also the seismic signatures of the OCTs show important differences. At the south, although several MCS dipping reflectors reach mantle depths, the WA data require reflections from the Moho to fit the observed amplitudes. At the central segment, the region of the OCT adjacent to the continental crust also generates PmP phases, but further west no first order discontinuities have been reported and the transitional crust velocity increases smoothly to reach mantle velocity. The former differences favor a two pulse continental breakup instead of a relatively uniform propagation.

NEW SEISMIC REFLECTION IMAGES OF THE ZONE OF EXHUMED CONTINENTAL MANTLE (ZECM) AT THE IBERIAN ABYSSAL PLAIN OCEAN-CONTINENT TRANSITION

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Over the past few years, the interpretations on the nature of the basement at the Ocean-Continent Transition in the Iberian Abyssal Plain have changed considerably. Presently, the transition from thinned continental to oceanic crust is interpreted as a ZECM due to delamination and removal of continental crust, by low angle detachment faulting, in an essentially magmatically starved environment. The ZECM was targeted by a MCS reflection and wide angle refraction survey in the summer of 2006 in the scope of the Portuguese Continental Shelf Extension Program. Nearly 1600 km of 2D MCS reflection lines were performed, along E-W and N-S directions and tie with existing academic and industry surveys. The lines were acquired serving a two fold purpose: 1: constrain the sediment thickness 2; characterize the basement and intra-basement structure at the Iberian Abyssal Plain and Southern edge of the Galicia Bank and Interior Basin. The layout therefore consisted on a 8km long streamer and an array of bolt long-life air guns (5720 cu.in.). In order to record deep reflections the record length was set to 18s. The E-W lines were Kirchoff pre-stack depth migrated (PSDM) using Paradigm's Geodepth software. Results so far, show a clear improvement with respect to the original time migrated lines, especially for the deeper sections. We present a comparison between interpretations based on this enhanced PSDM images and existing tectonic models for this segment of the West Iberian Margin.

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THE INTERPLAY OF OCT AND MIOCENIC DEFORMATION IN THE TAGUS ABYSSAL PLAIN

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 Transition -
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 Académie des
 Sciences, Paris,
 September, 2007.*

The West Iberian margin suffered a main compressive event during Miocenic times. The deformation that this event produced is clearly identified on its southern segment and seems to be concentrated in two main areas, within the short OCT and further west near the base of the Tore-Madeira rise. We concentrate on a geological transect of the crust and upper mantle structure in the TAP, extending from the un-thinned continental crust in the east to the oceanic crust in the west. This cross-section is constrained by one deep-penetrating MCS profile - IAM5, coincident recordings of refractions and wide-angle reflections by OBS's and land stations, 2-D modelling of gravity and magnetic data. The effect of the Miocenic deformation in the TAP is studied using finite element models of flexure that incorporate realistic rheologies. Several hypothesis about the thermo-mechanical structure of the OCT are tested and compared to the observed pattern of deformation.

STRUCTURE AND EVOLUTION OF THE TAGUS ABYSSAL PLAIN

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The opening of the North Atlantic Ocean is registered along the Newfoundland and West Iberia margins, perhaps the best studied nonvolcanic margins of the world (e.g. Boillot et al., 1987; Reid, 1994; Reston et al., 1995; Pickup et al., 1996; Dean et al., 2000; Withmarsh et al., 2001; Funk et al., 2003; Hooper et al., 2004; Shillington et al., 2006). Striking differences occur in the structure of this conjugated system. In Newfoundland extended continental crust thins abruptly with few crustal-scale normal faults, while Iberia continental crust is dominated by seaward dipping normal faults and high angle faults that terminate at low angle-surfaces interpreted as detachment faults. The character of the transition zone is also remarkably different, having in Newfoundland margin been interpreted as thinned continental crust emplaced during the late stages of rifting, while in the Galicia Bank and Iberian Abyssal Plain (IAP) it is interpreted as a varying width zone of exhumed continental mantle (ZECM). These contrasts favour asymmetric models of continental breakup and complex transitions from late stage continental rifting to oceanic accretion.

Spatio-temporal variations in the rifting process also appear to exist between the Iberian Abyssal Plain, in the north, and the Tagus Abissal Plain (TAP), in the south of the Iberian margin. A geological transect of the crust and upper mantle structure in the TAP, extending from the un-thinned continental crust in the east to the oceanic crust in the west, has been recently published (Afilhado, 2006). This cross-section is constrained by one deep-penetrating MCS profile - IAM5, coincident recordings of refractions and wide-angle reflections by OBS's and land stations, 2-D modelling of gravity and magnetic data. The knowledge of the deep structure obtained is comparable to the one already available in the Iberia Abyssal Plain where 2 Legs of the Ocean Drilling Program took place.

Comparing the TAP and IAP crustal structures we find several differences. At the TAP a short (~30km) segment of transitional crust contrasts to the wide ZECM (~150km) found at the IAP. Although a large body of exhumed mantle at the ocean-continent transition is hardly supported by the potential dataset, the eastern 35km segment of the

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TAP is a mass excess segment, bordered by positive magnetic anomalies, in good agreement with an intruded and partly ultramafic transitional crust, as suggested by the seismic data. Furthermore, the lower transitional crust extends from the TAP to the continental slope, while at the northern segment of the margin the ZECM is confined to the abyssal plain.

According to the last exhaustive work on seismic stratigraphy of the region (Mougenot, 1989), the margin suffered a main compressive event during Miocenic times. The deformation that this event produced is clearly identified on IAM5 profile and seems to be concentrated in two main areas, within the short transitional domain and further west near the base of the Tore-Madeira rise.

Other important event that affected this region is the sub-aerial volcanism at Mo times that formed the Madeira Tore Rise and the well known J magnetic anomaly (Tucholke and Ludwig, 1982). The thermo-mechanical effect of such event has not yet been addressed. Thus, both the Miocenic compression and the emplacement of the Tore-Madeira need to be taken into account in order to estimate as accurately as possible the evolution of the geometry of the rifted basin.

To study the thermo-mechanical evolution of the margin we follow the modelling formulation of Behn et al. (2002). We developed a lagrangian visco-plastic finite element program that incorporates strain-rate softening to simulate the rate-dependence of frictional strength observed in the laboratory. In this approach non-linear rheology is simulated by iterative linearization of the effective viscosity. A frictional failure criterion is used to bound the maximum principle shear stress in each element. The time-dependence of the frictional strength is simulated by introducing a strain-rate dependence on the cohesion coefficient. Forcing of the model is implemented through velocity boundary conditions and gravitational body forces. The modelling results are a proxy for the initial pattern of deformation that will form in response to a given set of thermal and rheological conditions. The advantage of this formulation is that it predicts zone of localized deformation (high strain rate) that can be considered analogous to faults. The method has been successfully applied to explain the spatio-temporal evolution of deformation in the North Sea (Cowie et al., 2005). By using these numerical tools we expect to assess the degree of coupling between basement and near surface deformation and determine the thermal conditions and boundary forces that cause zones of strain localization consistent with the fault patterns observed in the TAP transect. A well constrained picture of the evolution of the south segment of the West Iberia margin will also contribute to a better understanding of the North Atlantic rifting process.

CONSTRAINING THE TECTONIC- -THERMAL EVOLUTION OF THE SW PORTUGUESE MARGIN

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The TAP and adjacent continental margin are today considered passive, but they suffered in the past two major tectonic events. The first occurred during the emplacement of the Tore-Madeira Rise (~90Ma). The second occurred during the Miocene, when the whole SW Iberian Margins was submitted to a strong compressional phase. In order to understand the early stages of the formation of the margin we propose to explore the effects of these two tectonic events on the deep structure of the margin. Both these tectonic events were recorded in the stratigraphy of the TAP. In 2006 a geological transect of the crust and upper mantle structure in the Tagus Abyssal Plain (TAP) was published, extending from the un-thinned continental crust in the East to the typical oceanic crust in the West. This cross-section is constrained by one deep-penetrating MCS profile, coincident recordings of refractions and wide-angle reflections by OBS's and land stations, 2-D modelling of gravity and magnetic data. The knowledge of the deep structure obtained is comparable to the one already available in the Iberia Abyssal Plain where 2 Legs of the Ocean Drilling Program took place. Using this state-of-the-art geological cross-section, we will study the main tectonic episodes that affected the lithosphere in the TAP using 2D finite-element numerical models. The formulation couples strain localization mechanisms that simulate brittle fault growth and temperature dependent viscous deformation. The modelling will provide constrains on the tectonic-thermal evolution of the SW Portuguese margin, particularly on the amount of lithospheric uplift associated with the emplacement of the Tore-Madeira Rise, the amount of Miocenic compression, the role of pre-existing weakness zones on the deformation pattern, and the degree of coupling between basement and near surface deformation.

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APLICAÇÃO DE GEOSSINTÉTICOS EM TÚNEIS A CÉU ABERTO

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Exigências de funcionalidade, longevidade e segurança são algumas das muitas razões pelas quais se justifica a impermeabilização dos túneis executados a céu aberto. Nos últimos dez anos, a maioria dos túneis executados a céu aberto, construídos em Portugal, tem sido provida de sistemas de impermeabilização com geomembranas e drenagem associada com materiais geossintéticos. A preferência por estes materiais prende-se com a sua boa adaptabilidade aos mais variados tipos de suporte, pela instalação rápida, fiabilidade e boa relação - qualidade preço.

A presente comunicação tem por objectivo a apresentação dos sistemas de impermeabilização e drenagem associada mais comuns nas obras subterrâneas construídas a céu aberto, acima do nível freático, bem como alguns dos detalhes construtivos a eles associados. Serão apresentados alguns casos de obra com o objectivo de mostrar as metodologias de instalação dos respectivos sistemas de impermeabilização e drenagem associada e alguns dos cuidados básicos a serem observados.

ATERROS DE RSU EM PORTUGAL: ANÁLISE E PERSPECTIVAS FUTURAS

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Em Portugal, nos últimos 10 anos, houve uma grande mudança na política de gestão de resíduos, tendo-se encerrado as lixeiras existentes e construído em sua substituição cerca de 40 aterros de RSU. Numa altura em que os primeiros destes aterros começam a atingir o limite da sua vida útil, sendo por isso necessário iniciar uma nova fase de construções deste tipo de infra-estruturas e dada a importância que o desempenho dos geossintéticos têm na eficácia do funcionamento dos sistemas de confinamento e de cobertura dos aterros de RSU, considerou-se importante apresentar essa experiência e retirar alguns ensinamentos, nomeadamente no que respeita aos materiais utilizados, às técnicas empregues e aos problemas encontrados. O objectivo deste trabalho é o de permitir por um lado uma melhor compreensão da natureza, frequência e significado dos problemas identificados e por outro apresentar algumas recomendações para os minimizar.

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RATE OF LIQUID FLOW THROUGH COMPOSITE LINERS DUE TO DEFECTS IN THE GEOMEMBRANE: RECENT ADVANCES

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This paper presents the recent advances on the existing methods for evaluating the rate of advective flow through composite liners. The advective flow is due to the existence of defects in the geomembrane and depends on the features of interface between the geomembrane and the underlying liner, which can be expressed either by the interface transmissivity, or by contact conditions. Direct methods (laboratory tests), and indirect methods (analytical equations, empirical and semi-empirical equations and numerical analysis) are addressed. The main goal of this work is to provide design engineers with a review of the tools currently available to calculate the advective flow through composite liners.

PLANO DE GARANTIA DE QUALIDADE DA CONSTRUÇÃO PARA GEOSSINTÉTICOS: SUGESTÕES PARA O FUTURO

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Nos aterros de RSU tem-se assistido a um aumento sistemático da aplicação de geossintéticos pelas inúmeras vantagens que apresentam relativamente aos materiais minerais, não só por permitirem aumentar a capacidade de armazenamento de resíduos, mas também por serem mais homogêneos e de mais rápida e fácil colocação. No entanto, a experiência tem demonstrado que o seu desempenho é muito influenciado pelo modo de instalação, sendo particularmente sensíveis ao punçoamento, verificando-se os principais danos durante a fase de construção. É por isso amplamente reconhecido que a garantia de qualidade da construção (GQC) e a qualidade do controlo da construção (QCC) são determinantes para a qualidade do desempenho dos aterros de resíduos. Salvo raras exceções, os procedimentos de GQC, no que se refere aos geossintéticos, têm permanecido praticamente inalterados durante a última década. Considerou-se por isso importante fazendo uso da experiência acumulada, analisar a adequação dos métodos usualmente empregues na avaliação da qualidade de aplicação dos geossintéticos e, tendo igualmente em consideração as novas tecnologias, propor as alterações julgadas convenientes, para melhorar a eficácia dos planos de GQC nomeadamente no que respeita aos geossintéticos.

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ENSINAMENTOS RECENTES SOBRE O DESEMPENHO DOS GEOSSINTÉTICOS

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Este artigo descreve, em primeiro lugar, os tipos de confinamento basal e de cobertura dos aterros de resíduos. Seguidamente apresenta e comenta os principais aspectos que podem comprometer o desempenho das barreiras geossintéticas (geomembranas e geossintéticos bentoníticos) nos sistemas de confinamento. Entre os aspectos em análise incluem-se a migração de contaminantes através das barreiras geossintéticas (por difusão e por advecção), a durabilidade das geomembranas e dos geossintéticos bentoníticos, a protecção da geomembrana e as dobras na geomembrana.

DEGRADAÇÃO POR CARUNCHO GRANDE EM ESTRUTURAS DE MADEIRA ANTIGAS: APRESENTAÇÃO DE UM CASO DE ESTUDO

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Uma correcta remodelação ou reabilitação de um edifício deve ser precedida por uma observação atenta que permita o diagnóstico das suas deficiências, danos estruturais e degradação sofrida ao longo do tempo. Só depois de realizado um apurado estudo de inspecção e diagnóstico, se deverá concluir pela remoção ou não das suas peças ou parte delas, especialmente no que se refere aos elementos em madeira. A madeira, como material estrutural fortemente presente nas construções anteriores a 1940, exhibe por vezes diversos sinais de degradação derivada não apenas do facto de ser um material orgânico, mas sobretudo da escassez de acções de manutenção e da falta de compreensão das suas características ao longo do tempo, com especial ênfase para as últimas décadas.

Nesse sentido, o presente artigo fornece uma orientação sumária para a compreensão dos fenómenos de degradação de madeira por carunchos e respectiva sintomatologia. Apresenta também uma breve introdução aos métodos de ensaio não destrutivos actualmente disponíveis para suporte a acções de inspecção *in situ*.

Como forma ilustrativa de transmissão de conhecimento sobre o trabalho de inspecção e diagnóstico a aplicar em obra, apresenta-se um caso real de um edifício antigo degradado cuja patologia foi identificada e estudada. Descreve-se a situação de degradação encontrada com especial relevo para a degradação por caruncho grande, enunciam-se os critérios que presidiram à selecção dos métodos utilizados, apresentam-se graficamente os resultados obtidos, faz-se a sua análise crítica e respectiva inter-relação.

Esta comunicação resulta do estudo para uma tese de doutoramento em desenvolvimento no LNEC, que pretende tratar laboratorialmente e *in situ*, as questões relativas à reabilitação de elementos estruturais em madeira que se encontrem degradados por agentes biológicos.

Palavras-chave: madeira, estruturas, caruncho grande, patologia, edifícios antigos.

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WATER RECYCLING AND REUSE IN EUREAU COUNTRIES: TRENDS AND CHALLENGES

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EUREAU is a non-profit Union of National Associations of Water Suppliers and Wastewater Services from EU and EFTA countries. EUREAU countries depend on appropriately treated wastewater to protect the environment and ensure that freshwater is available for all applications. Indirect water recycling and reuse through surface and groundwater bodies is common practice and public health is protected through potable water standards for centuries. Water recycling and reuse for non potable applications or potable substitution has been practiced in Europe since the Minoan era (ca. 5000 years ago). It has been also proven internationally in water stressed regions to be a drought proof source of water and one of the most effective water scarcity solutions. This paper considers: (a) the status of water recycling and reuse in EUREAU countries, (b) the major challenges, (c) the future views, and (d) successful examples wastewater recycling and reuse in Europe.

MODELAÇÃO DE CONSTRUÇÕES EM TERRA CRUA SUJEITAS À ACÇÃO SÍSMICA

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A utilização da terra tem servido não só para a construção de habitações rurais e urbanas mas também, para erguer grandes monumentos. Este tipo de construção deveu-se à grande carência habitacional e, esta está directamente relacionada com a escassez de recursos financeiros das populações, sendo de extrema importância a revitalização do uso da terra como material de construção. A terra será sempre um dos materiais contemplados na construção das habitações, devido à sua abundância, custo acessível, tradição e facilidade de execução. Mas os problemas energéticos, ambientais, ecológicos e económicos sentidos a nível mundial, conduzem a uma mudança de mentalidades nos escalões privilegiados das sociedades desenvolvidas. A terra crua como material de construção deixa de ser sinónimo de desconforto e pobreza para começar a ser visto como um material alternativo e valorizado. Actualmente, por todos os continentes, está em curso um revivalismo da arquitectura de terra.

A presente comunicação tem como objectivo descrever duas modelações efectuadas em elementos finitos com Sólidos, usando o programa de software para Análise Estrutural - STRUCTURAL ANALYSIS SAP 2000, versão 10.0.1. Modelações estas, que pretendem simular o comportamento de edificações em Terra Crua quando sujeitas a um sismo.

Após uma análise dos resultados obtidos através das modelações, concluiu-se que a utilização de diversos materiais distintos, influencia em muito no comportamento destas construções, quando sujeitas a uma acção sísmica.

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TSUNAMI VULNERABILITY ASSESSMENT OF CASABLANCA – MOROCCO, PILOT STUDY

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In this study we present a preliminary evaluation of the tsunami vulnerability of Casablanca area (Morocco) and the expected inundation from a tsunami generated in the North East Atlantic area in the Gulf of Cadiz using a combination of numerical modeling and GIS tools. The study area is the intensively occupied area of the Casablanca Harbor, a location that may be considered as one of the most vulnerable areas to tsunami hazard, along Morocco Atlantic coast, due to its location close to the source of moderate and strong magnitude earthquakes, the extension of low flat areas close to the sea and the existence of dwellings characterized by unstructured constructions. To study vulnerability and inundation we considered geomorphologic and artificial elements as well as the existence of defensive constructions. The inundation zone was divided in for sub-zones according to their height above sea level; the buildings were classed according to: building material, number of floors, conditions of foundation soil. The study area presents a large variety of constructions: 1 storey buildings of 2- 2.5m height, houses and stores of the ancient medina and some modern buildings. The results are presented, using GIS and show a preliminary “picture” of built stock behaviour in case of tsunami for Casablanca. The results clearly demonstrate.

COMPORTAMENTO DAS CONSTRUÇÕES EM TERRA QUANDO SUJEITAS A UM SISMO

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As tecnologias tradicionais de construção com terra são variadas, com inúmeras adaptações à qualidade da terra, à identidade das culturas e aos lugares, de acordo com as diferentes experiências e com as formas de pensar da sociedade e da época onde se integram.

Nas construções de pequeno porte, as paredes em conjunto com os pavimentos e a cobertura desempenham, simultaneamente, funções resistentes e estruturais (para cargas verticais e horizontais). Nas construções em terra, é o comportamento das paredes que tem um carácter decisivo no comportamento global. Estas construções funcionam por gravidade, pelo que as suas paredes apresentam uma razoável, ou até mesmo boa, resistência a esforços de compressão vertical por serem muito espessas. Pelo contrário, a capacidade das paredes para suportar cargas horizontais, nomeadamente as de origem sísmica, é muito variável, podendo ir desde a total inaptidão até a uma resistência satisfatória em construções de pequeno porte, conseguida através de soluções estruturais sísmo-resistentes.

Os danos provocados pelos sismos nas edificações dependem: da intensidade do sismo; da resistência da edificação; da qualidade da construção e de determinadas características da edificação, tais como a distribuição da massa, a altura, o peso das paredes e da cobertura. Pode-se minimizar a influência da acção sísmica nestas construções, através de uma correcta concepção da estrutura na fase de projecto quer da qualidade da construção.

Não existe até à data nenhuma regulamentação para as construções em terra crua, já que apenas as estruturas de betão armado e as metálicas estão contempladas nos regulamentos estruturais Portugueses. Existe assim a necessidade de criar normas para as construções em terra crua, tendo em conta as características específicas deste material.

Neste artigo, será feito um levantamento do comportamento das edificações de terra quando sujeitas a um sismo.

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APLICABILIDADE DE MÉTODOS DE ESTUDO DA COMPOSIÇÃO DE BETÃO AUTO-COMPACTÁVEL (BAC)

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2007, C21, pp. 53.*

O presente artigo tem como objectivo apresentar os resultados obtidos na campanha experimental para o estudo de verificação da aplicabilidade técnica de dois métodos de cálculo de composição de betão auto-compactável - BAC - propostos por investigadores nacionais em trabalhos anteriores.

Com o referido estudo, pretendeu-se, através dos métodos em análise, identificar o método que permite de um modo mais simples, sem necessidade de recorrer a um grande número de amassaduras experimentais, obter as características requeridas aos BAC, tanto no estado fresco como no estado endurecido.

Da análise de resultados efectuada, é possível a comparação entre os métodos estudados e verificação da sua aplicabilidade, bem como identificar quais os factores que condicionam o processo de cálculo de amassaduras de BAC.

Palavras-chave: Betão auto-compactável e métodos de estudo de composição.

AVALIAÇÃO DE TÉCNICAS CONSTRUTIVAS UTILIZADAS NA REABILITAÇÃO SÍSMICA DE EDIFÍCIOS EM ALVENARIA DE PEDRA

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Mestrado em: Construção

Grau Concedido por: Instituto Superior Técnico

Orientadores: Doutor Fernando António Baptista Branco

Provas Concluídas em: 3 de Maio de 2007

Existem diversas soluções para reforço sísmico de estruturas em alvenaria de pedra argamassada, que podem ir desde a introdução de novos elementos estruturais até à execução de pequenos reforços locais, passando pela criação de mecanismos de dissipação de energia. A escolha do processo a adoptar depende de diversos factores, tais como:

- | tipologia do edifício a reforçar;
- | tipo de utilização e importância do mesmo;
- | estado de conservação;
- | disponibilidade financeira.

Pretendeu-se, com este trabalho, contribuir para uma escolha mais correcta da técnica de reabilitação estrutural a adoptar, tendo em conta o risco sísmico que abrange grande parte do nosso país.

Elaborou-se então um estudo que inclui a compreensão e a forma de execução das técnicas de reabilitação sísmica habitualmente utilizadas em edifícios antigos, suas vantagens e desvantagens, e por fim, estudou-se um edifício, sua modelação num programa de cálculo automático, simulação de diversas técnicas de reforço no dito edifício e análise das alterações introduzidas por cada uma delas no mesmo.

Palavras-chave: reabilitação; modelação; alvenaria de pedra; sísmica; reforço; edifício antigo.

BETÕES EXECUTADOS COM AGREGADOS FINOS RECICLADOS DE BETÃO

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Mestrado em: Construção

Grau Concedido por: Instituto Superior Técnico

Orientadores: Jorge Manuel Lopes Caliço de Brito

Provas Concluídas em: 3 de Maio de 2007

A evolução da civilização trouxe consigo problemas ambientais graves. Não só a emissão de gases potenciadores do efeito de estufa atingiu limites perigosos, como também o consumo de recursos naturais está prestes a causar um colapso ambiental generalizado.

O crescimento da população mundial, associado aos êxodos em massa das populações para os centros urbanos, está a causar um forte crescimento da construção, que é uma das indústrias ecologicamente menos eficientes que existe. Com esse crescimento, não só o consumo de recursos, renováveis e não renováveis, cresce, acompanhado das inevitáveis emissões atmosféricas, como também a produção de resíduos acompanha a tendência.

Com o sentido de inverter esse aumento, existem actualmente esforços para promover a eficiência ecológica na indústria da construção, sendo a reutilização dos resíduos da construção e demolição, uma das vertentes exploradas. Nesta, a utilização de agregados reciclados como substitutos dos seus congêneres naturais é tomada como uma das formas mais salutares de contribuir para uma melhor sustentabilidade da construção. No entanto, a reciclagem de agregados para uso em betão tem-se concentrado quase unicamente na parcela grossa dos mesmos, rejeitando a fracção fina. Esta rejeição advém, fundamentalmente, do facto de os materiais finos reciclados serem francamente porosos, causando reduções de desempenho dos betões com eles executados.

Nesta investigação, pretendeu-se avaliar o comportamento de betões executados com agregados finos reciclados de betão, de modo a poder estabelecer a sua viabilidade prática, permitindo, deste modo, reduzir os consumos de areias, cuja extracção acarreta graves custos ambientais.

MÉTODOS DE ESTUDO DA COMPOSIÇÃO DE BETÃO AUTO-COMPACTÁVEL (BAC) – VERIFICAÇÃO DA SUA APLICABILIDADE TÉCNICO-ÉCONÓMICA

Silva, Pedro Miguel Soares da

Mestrado em: Construção

Grau Concedido por: UTL – Instituto Superior Técnico

Orientadores: Doutor Jorge Manuel Calião Lopes de Brito (Orientador) e

Mestre João Manuel Barrento da Costa (Co-orientador)

Provas Concluídas em: 12 de Dezembro de 2007

A crescente escassez de mão-de-obra especializada no Japão, no início da década de 80, motivou uma procura da melhoria da durabilidade das estruturas, independentemente da qualidade dos trabalhos de compactação, intensificando-se, assim, os estudos para a obtenção de betões que dispensassem qualquer método de compactação. Esses betões designam-se por auto-compactáveis – BAC (em inglês: “Self Compacting Concrete” – SCC).

É considerado por muitos como o desenvolvimento mais revolucionário das últimas décadas na área da construção civil, essencialmente devido ao facto de envolver um novo processo de produção e colocação do betão em obra, o qual assenta na eliminação da vibração de forma a aumentar a qualidade do produto final com uma eventual diminuição do custo global da betonagem.

Não obstante, apesar de possuir já uma vasta utilização a nível mundial, não apresenta ainda consumos equivalentes aos do betão convencional. Vários factores contribuem para tal facto, dos quais, a falta de métodos de estudo da composição de amassaduras expeditos e adequados à obtenção de uma mistura satisfatória que dê resposta a requisitos tanto no estado fresco como endurecido continua a ser um dos principais obstáculos à implementação deste novo material.

Por outras palavras, não se tem prestado a atenção adequada ao processo de cálculo de amassaduras visando a obtenção de determinado valor de resistência mecânica, havendo sempre a necessidade de recorrer a um elevado número de amassaduras experimentais de modo a aferir o valor médio da resistência mecânica expectável.

Nesse sentido, o presente trabalho teve como objectivo avaliar a aplicabilidade técnico-económica de dois métodos de cálculo de composição de BAC propostos por investigadores nacionais em trabalhos anteriores.

Com o referido estudo, pretendeu-se, através dos métodos em análise, identificar o método que permite obter as características requeridas aos BAC, tanto no estado fresco como no endurecido de um modo mais simples, sem necessidade de recorrer a um grande número de amassaduras experimentais.

Da análise de resultados efectuada, é possível a comparação entre os métodos estudados e a verificação da sua aplicabilidade tanto técnica como económica, bem como a identificação de quais os factores que condicionam o processo de cálculo de amassaduras de BAC.

Palavras-chave: betão auto-compactável (BAC), métodos de estudo de composição, viabilidade técnico-económica.



02

ENGENHARIA DE ELECTRÓNICA DE TELECOMUNICAÇÕES E DE COMPUTADORES

Anuário Científico 2007

ISEL

ADAPTIVE MOTION ESTIMATION PROCESSOR FOR AUTONOMOUS VIDEO DEVICES

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Motion estimation is the most demanding operation of a video encoder, corresponding to at least 80% of the overall computational cost. As a consequence, with the proliferation of autonomous and portable handheld devices that support digital video coding, data-adaptive motion estimation algorithms have been required to dynamically configure the search pattern not only to avoid unnecessary computations and memory accesses but also to save energy. This paper proposes an application-specific instruction set processor (ASIP) to implement data-adaptive motion estimation algorithms that is characterized by a specialized datapath and a minimum and optimized instruction set. Due to its low-power nature, this architecture is highly suitable to develop motion estimators for portable, mobile, and battery-supplied devices. Based on the proposed architecture and the considered adaptive algorithms, several motion estimators were synthesized both for a Virtex-II Pro XC2VP30 FPGA from Xilinx, integrated within an ML310 development platform, and using a StdCell library based on a 0.18 μm CMOS process. Experimental results show that the proposed architecture is able to estimate motion vectors in real time for QCIF and CIF video sequences with a very low-power consumption. Moreover, it is also able to adapt the operation to the available energy level in runtime. By adjusting the search pattern and setting up a more convenient operating frequency, it can change the power consumption in the interval between 1.6mW and 15mW.

Publicado em:

EURASIP Journal on Embedded Systems - Special Issue on Embedded Systems for Portable and Mobile Video Platforms, 2007, 57234, 1-10

RECONFIGURABLE ARCHITECTURES AND PROCESSORS FOR REAL-TIME VIDEO MOTION ESTIMATION

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*Journal of Real-Time
Image Processing -
Special issue on Field-
Programmable
Technology, 2007, 11-4,
191-205*

With the recent proliferation of multimedia applications, several fast block matching motion estimation algorithms have been proposed in order to minimize the processing time in video coding. While some of these algorithms adopt pre-defined search patterns that directly reflect the most probable motion structures, other data-adaptive approaches dynamically configure the search pattern to avoid unnecessary computations and memory accesses. Either of these approaches leads to rather difficult hardware implementations, due to their configurability and adaptive nature. As a consequence, two different but quite configurable architectures are proposed in this paper. While the first architecture reflects an innovative mechanism to implement motion estimation processors that support fast but regular search algorithms, the second architecture makes use of an application specific instruction set processor (ASIP) platform, capable of implementing most data-adaptive algorithms that have been proposed in the last few years. Despite their different natures, these two architectures provide highly configurable hardware platforms for real-time motion estimation. By considering a wide set of fast and adaptive algorithms, the efficiency of these two architectures was compared and several motion estimators were synthesized in a Virtex-II Pro XC2VP30 FPGA from Xilinx, integrated within a ML310 development platform. Experimental results show that the proposed architectures can be easily reconfigured in run-time to implement a wide set of real-time motion estimation algorithms.

OPTICAL READOUT IN PINPI'N AND PINI'P IMAGERS: A COMPARISON

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Optimized a-SiC:H multilayer devices based on two different tandem configurations (TCO/pinpi'n/TCO and TCO/pini'p/TCO) are compared and tested for proper image recognition and color separation process using an optical readout technique. In both configurations the doped layers are based on a-SiC:H to increase image resolution and to prevent image blurring. To profit from the light filtering properties of the active absorbers, the intrinsic layer of the front diode (i layer) is based on a-SiC:H and the back one (i' layer) on a-Si:H. The effect of the applied voltage on the color selectivity is discussed. Results show that the relative spectral response curves demonstrate rather good separation between the red, green and blue basic colors. Combining the information obtained under positive and negative applied bias a colour image is acquired, using the same optical technique either in pinpi'n or in the pini'p configuration, without colour filters or pixel architecture.

Publicado em:

*Actas da Mat. Res.
Soc. Spring Meeting,
Francisco, 9 a 13 de
Abril de 2007,
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PRELIMINARY RESULTS ON LARGE AREA X-RAY A-SIC: H MULTILAYER DETECTORS WITH OPTICALLY ADDRESSED READOUT

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This paper investigates the feasibility of using a large area image sensor with an optically addressed readout for medical X-ray diagnostic imaging. The device prototype comprises a multilayer glass/ZnO:Al/p (a-SiC:H)/i (a-Si:H)/ n (a-SiC:H)/ i(a-Si:H)/p (a-SiC:H)/ a-SiNx/ITO structure coupled to a scintillator layer. Here, the p-i-n-i-p structure works in both sensing and switching modes depending on the biasing conditions. A numerical simulation is used to optimize the semiconductor layer thicknesses in order to achieve a photocurrent matching between back-to-back diodes in switching mode. The charge carrier transport within the p-i-n-i-p structure is also analyzed under different electric and optical biasing conditions. A physical model supports the results.

Publicado em:

Actas da Mat. Res. Soc. Spring Meeting, Francisco, 9 a 13 de Abril de 2007, vol. 989, A19-02.

MODELING THE LASER SCANNED PHOTODIODE S-SHAPED J-V CHARACTERISTIC

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The devices analyzed in this work present an S-shape J-V characteristic when illuminated. By changing the light flux a non linear dependence of the photocurrent with illumination is observed. Thus a low intensity light beam can be used to probe the local illumination conditions, since a relationship exists between the probe beam photocurrent and the steady state illumination. Numerical simulation studies showed that the origin of this S-shape lies in a reduced electric field across the intrinsic region, which causes an increase in the recombination losses. Based on this, we present a model for the device consisting of a modulated barrier recombination junction in addition to the p-i-n junction. The simulated results are in good agreement with the experimental data. Using the presented model a good estimative of the LSP signal under different illumination conditions can be obtained, thus simplifying the development of applications using the LSP as an image sensor, with advantages over the existing imaging systems in the large area sensor fields with the low cost associated to the amorphous silicon technology.

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Actas da Mat. Res. Soc. Spring Meeting, Francisco, 9 a 13 de Abril de 2007, vol. 989 A12-04.

PHOTOCURRENT PROFILE IN A-SiC:H MONOLITHIC TANDEM PINPIN AND PINIP PHOTODIODES

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Publicado em:
*Actas da Mat. Res.
Soc. Spring Meeting,
Francisco, 9 a 13 de
Abril de 2007,
vol. 989, A18-14.*

We present in this paper results about the analysis of photocurrent and spectral response in a-SiC:H/ a-Si:H pinpin and pinip structures. Our experiments and analysis reveal the photocurrent profile to have a strong nonlinear dependence on the externally applied bias and on the light absorption profile, *i.e.* on the incident light wavelength and intensity. Our interpretation points out the cause of such effect to a self biasing of the junctions under certain unbalanced light generation of carriers and to an asymmetric reaction of the internal electric fields to the externally imposed bias. The possibility to relate such a behavior to the light intensity and wavelength indicates realistic hypothesis of using these structures and this effect for color recognition sensors. We present results about the experimental characterization of the structures and numerical simulations obtained with the program ASCA. Considerations about electrical field profiles and inversion layers will be taken into account to explain the optical and voltage bias dependence of the spectral response. Our results show that in both structures the application of an external electrical bias (forward or reverse) mainly influences the field distribution within the less photo excited sub-cell.

SPIN POLARIZATION OF DILUTED MAGNETIC SEMICONDUCTORS UNDER THE IMPURITY PHOTOEXCITATION

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- 5 Electronics Telecommunications and Computer Dept., ISEL, Lisbon, Portugal
- 6 CFIF, Instituto Superior Técnico, Lisboa, Portugal

We propose a set of kinetic equations to describe spin polarization of band electrons in a semiconductor doped with elements with unfilled 3d or 4f shells, subject to polarized light. Stationary solutions of these equations are also derived. The influence of light intensity, its polarization type (left- and right-handed circular or linear), and magnetic impurity concentration NT on the polarization degrees of band electrons p_e and impurity ions $\rho_{\tilde{N}}$ is investigated. It is shown that p_e under the influence of left-handed circularly polarized light increases with the light intensity and impurity concentration. In the case of right-handed circularly polarized wave, the conduction electron spin polarization decreases, whereas under the influence of linearly polarized light it is almost independent of both ρ_0 and NT . The calculations of p_e as a function of light polarization type are in good agreement with available data on III-V diluted magnetic semiconductors.

Publicado em:

Actas da Mat. Res. Soc. Spring Meeting, Francisco, 9 a 13 de Abril de 2007, vol. 999, K05-04.

MODELING AND CHARACTERIZATION OF THE HYDROGENATED AMORPHOUS SILICON METAL INSULATOR SEMICONDUCTOR PHOTODETECTORS FOR DIGITAL RADIOGRAPHY

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Because of the inherent desired material and technological attributes such as low temperature deposition and high uniformity over large area, the amorphous silicon (a-Si:H) technology has been extended to digital X-ray diagnostic imaging applications. This paper reports on design, fabrication, and characterization of a MIS-type photosensor that is fully process-compatible with the active matrix a-Si:H TFT back-plane. We discuss the device operating principles, along with measurement results of the transient dark current, linearity and spectral response.

Publicado em:

*Actas da Mat. Res.
Soc. Spring Meeting,
Francisco, 9 a 13 de
Abril de 2007,
vol. 989, A12-06.*

COLOUR SENSITIVE DEVICES BASED ON DOUBLE P-I-N-I-P STACKED PHOTODIODES

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In this work, we report on an amorphous silicon based image sensor with a bias voltage controllable spectral response characteristics. This multilayered device is composed by two stacked p-i-n-i-p structures produced by plasma enhanced chemical vapour deposition on a glass substrate and sandwiched between two transparent conductive oxide electrodes with a patterned molybdenum layer between the sensing and switching structures. Optical readout technique is used for image readout. Device performances have been evaluated from the current-voltage characteristics and spectral response measurements performed for the p-i-n-i-p test structures and stacked device. It is demonstrated that the device is sensitive to blue-green or red light depending on polarity of the bias voltage enabling the detection of colour images. Device design is discussed and supported by a numerical simulation.

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Thin Solid Films,
2007, 515, 7526-7529

BIAS SENSITIVE MULTISPECTRAL STRUCTURES FOR IMAGING APPLICATIONS

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Thin Solid Films,
2007, 515, 7566-7570

In this paper we present results on the optimization of an pinpiin' type a-Si:H based three color detector with voltage controlled spectral sensitivity. The sensor element was fabricated on a glass covered with Indium Tin Oxide (ITO) and consists of a p-i-n a-SiC:H multilayer structure which faces the incident illumination, followed by a-SiC:H (-p)/a-SiC:H(-i)/a-Si:H(-i')/a-SiC:H(-n')/ITO heterostructure, that allows the optically addressed readout.

Results show that this approach leads to regionally different collection parameters resulting in multispectral photodiodes. In the polychromatic operation mode different sensitivity ranges are programmed by switching between different biases so that the basic colors can be resolved with a single device. Positive bias is needed under blue irradiation and moderated reverse bias under green. The threshold voltage between green and red sensitivity depends on the thickness of the bottom a-SiC:H (-i) layer, and corresponds to the complete confinement of the absorbed green photons across the pinpi sequence. As the thickness of the a-Si:H i'-layer increases, the self-reverse effect due to the front absorption will be balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias.

The various design parameters are discussed and supported by a 2D numerical simulation.

ACCREDITED VECTOR MAGNETOMETER CALIBRATION FACILITY

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 Posio, P.¹; Nevanlinna, H.¹; Schmidt, W.¹;
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The paper describes the accredited magnetometer calibration facility of the Nurmijärvi Geophysical Observatory of the Finnish Meteorological Institute. The magnetometer calibration is part of the Magnetic Calibration and Test Laboratory of the observatory, which was accredited by the Finnish Accreditation Services (FINAS) in August 2007. The facility comprises a three-axes coil system installed in a non-magnetic building, temperature test system and an automatic control and measuring system. Both analog and digital outputs of magnetometers can be connected to the control electronics and the calibration procedure can be run fully automatic or with a predefined protocol. Accurate orientation with optical methods allows determination of the angles between magnetic and mechanical axes of the magnetometer. Experimental results of a calibration of a satellite magnetometer are included to demonstrate the calibration concept.

Publicado em:

Geophysica, 2007,
 43(1-2), 59-76.

A NOVEL VEHICULAR MOBILITY MODEL FOR WIRELESS COMMUNICATIONS

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Publicado em:
Wireless Personal Communications Journal, Springer Science+Business Media, Agosto de 2007, pp, 43: 1689-1703.

In this paper a novel realistic vehicular mobility model is introduced. It captures the moving-in-groups, conscious traveling, and introduces the concept of smart traveling while following drivers' social behavior extracted from inquiries and experimental traffic measurements. Under the model, a routing algorithm is considered. The routing algorithm minimizes the distance to a target on a step by step form, in every street crossing. This is done under a hierarchic street level structure that optimizes travel speed and quality. The mobility model was simulated and validated in a real mobility scenario using, as case study, the city of Lisbon. The correlation values (between simulated data and theoretical distributions), arrival to destination success rate and directional statistics produced satisfactory results. The model concept is perfectly generic and applicable to other locations, provided that the corresponding street database and vehicular traffic information are available. The model outputs several parameters, including sinuosity indicator and traffic load. The sinuosity indicator is a powerful parameter on the characterization of urban radio environments when mobility is used in wireless networks simulation. Vehicular traffic load analysis is also presented. It can be used in further work over wireless traffic modeling, on a street segment basis or on a AU (Analysis Unit) perspective.

HIGH-VOLTAGE LDMOS TRANSISTORS FULLY COMPATIBLE WITH A DEEP-SUBMICRON 0.35 μm CMOS PROCESS

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This work presents the design of LDMOS transistors fully compatible with standard CMOS process, only requiring mask layout manipulation. A conventional 0.35 μm CMOS process was elected to demonstrate the viability of the approach. The prototyped LDMOS transistor exhibits a breakdown voltage of 24V, which represents an improvement of 31% when compared with the high-voltage extended-drain NMOS available in the process library, while other static parameters remain in the same range. Furthermore, this solution enables the CMOS integration of a high-voltage pass-transistors, as a consequence of the formation of an isolated lightly doped p-type region inside the n-well.

Publicado em:
Microelectronics Journal, 2007, 38, 35-40.

Keywords: High-voltage CMOS; MOSFET switch; LDMOS.

A TECNOLOGIA MIMO COMO RESPOSTA AO AUMENTO DE CAPACIDADE EM REDES MÓVEIS 3.5G

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Publicado em:
*Ingenium -Revista
Ordem Engenheiros, II
série, nº 100,
Julho/Agosto 2007.*

Neste artigo é abordado a problemática de aplicação da tecnologia MIMO em redes 3.5G assumindo um cenário multi-utilizador. A capacidade de Shannon é utilizada como uma métrica a ser transmitida na ligação ascendente, e desempenha um papel fundamental na determinação do ritmo de transmissão, estimação da taxa de tramas perdidas e escalonamento, ao nível do Node B. Foram introduzidas duas técnicas de escalonamento, denominadas Fair Capacity e Maximum Capacity SBSA, que utilizam a transmissão da métrica de Shannon para a melhoria de desempenho do sistema.

COMPLETE DISTRIBUTED GARBAGE COLLECTION USING DGC-CONSISTENT CUTS AND .NET AOP SUPPORT

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The memory management of distributed objects, when done manually, is an error-prone task. It leads to memory leaks and dangling references, causing applications to fail. Avoiding such errors requires automatic memory management, called distributed garbage collection (DGC).

Current DGC solutions are either not safe, not complete or not portable to widely used platforms such as .NET. As a matter of fact, most solutions either run on specialized environments or require modifications of the underlying virtual machine (*e.g.* rotor, common language runtime (CLR)), hindering its immediate and widespread utilization. This study describes the design, architecture, implementation and performance measurements of a DGC algorithm for .NET that: (i) is complete, that is, capable of reclaiming both acyclic and cyclic garbage, while (ii) being portable in the sense that it neither requires the underlying virtual machine to be modified, nor source or byte-code modification. The distributed garbage collector was implemented on top of two implementations of the common language infrastructure (.NET virtual machine specification): CLR and shared source CLI, commonly known as Rotor. The implementation requires no modification of the environment, it makes use of the provided aspect-oriented functionalities, and the performance results are encouraging.

Publicado em:

IET Software, 2007,
1, (6), 263-279

MODELING AND OPTIMIZING ERGONOMIC ACTIVITIES IN AUTOMOBILE PRODUCT DEVELOPMENT

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*Proceedings of
International
Conference on
Ergonomics 2007,
December 3-5, 2007 in
Kuala Lumpur
Malaysia.*

We collect ergonomic rules and normative rules considerations for automobile business and modeled these activities with a special UML language created for automobile business, VDML (Vehicle Development Modeling Language). From these high level process vision integrated in the product development activity a wide variety of improvements can be achieved related with time reduction, activity process quality as well as use of past experience. Also we intend to define ergonomic associated templates, which reflect standard ergonomic job routines to be incorporated in CAD application and improve the ergonomics process reference points and also the process optimization reached thorough UML high level vision. In these process we define also a ontology for ergonomics (EOL – Ergonomics Ontology Language) based on the OWL (Ontology Web Language) standards.

Keywords: Ontology, Knowledge Retrieval, Collaboration, CAD, Ergonomic, Modeling.

MODELING DESIGN ACTIVITY IN AUTOMOBILE INDUSTRY

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Designing and consequent assembly of a new vehicle is a complex process as it requires close coordination and inputs from a number of disciplines in developing a number of systems and sub-systems in the vehicle that should fit within the confined vehicle space, function and provide the customers an acceptable combination of all relevant vehicle attributes. Understanding how these processes interact and how they are aligned with other while they should support the tasks involved in the conception of a new vehicle at a minimum time and cost. The first step to achieve this goal is the Modeling Business Process using UML (industry standard language).

Keywords: Automobile Design, Modeling, UML-Profile.

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*Proceedings of
International
Conference IFAC
Conference on Cost
Effective Automation
in Networked Product
Development and
Manufacturing,
October 2-5, 2007 in
Monterrey NL México.*

PARTS LIFE CYCLE ACTIVITIES ON AUTOMOTIVE INDUSTRY

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Parts life cycle in automobile industry involves several actors among different companies and also different management systems. Most of systems do not change automatic information and information access is limited due to systems restrictions. Life cycle of parts is extensive in some cases could take 20 years and in this paper we propose a business process description with UML and a central system with appropriate interfaces for different phase actors

Publicado em:

*Proceedings of IFAC,
Fourth Conference on
Management and
Control of Production
and Logistics,
September 27 – 30,
2007 em Sibiu,
Romania.*

Keywords: Process, Manufacturing, Logistics, Life Cycle, UML.

CREATE KAR SYSTEM

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This paper defines the system CREATE KAR (CK) system, an integrated CAD (Computer Aided Design) and CSCW (Computer Supported Collaborative Work) system, to better support the design process in industry, basically on the development of new products in the automobile sector. This system intends to reduce the lead time by providing and integrating flexible and efficient capabilities for testing early concepts from the ergonomic, surface analysis and normative points of view in automotive product development. Based on domain ontology and on information repository we define tools for knowledge management and retrieval of technical knowledge via models in new CAD environment, helping the users to perform their job. These characteristics will differentiate the project from a commercial PDM (Product Data Management) system, because this last one lacks of all intelligent rules which are able to extrapolate and make inference with historical surfaces and solutions that allow the generation of surfaces (technological, material, structural constraints), the use of ergonomics and homologation rules and also the automatic integration of automatic job routines in CAD.

Keywords: Ontology, Knowledge Repository, Collaboration, Optimization, CAD.

Publicado em:

Proceedings of 4th International CIRP-Sponsored Conference (DET2007), September 19-21, 2007 in Bath, United Kingdom.

MODELING PRODUCT ENGINEER AND MANUFACTURING ACTIVITY IN VEHICLE DEVELOPMENT PROCESS

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Designing and consequent assembling of a new vehicle is a complex process as it requires close coordination and inputs from a number of disciplines in developing a number of systems and sub-systems in the vehicle that should fit within the confined vehicle space, function and provide the customers an acceptable combination of all relevant vehicle attributes. Understanding how these processes interact and how they are aligned with other while they should support the tasks involved in the conception of a new vehicle at a minimum time and cost is a difficult task. The first step to achieve this goal is the definition of a new UML profile (called VDML, Vehicle Development Modeling Language) based on the extension mechanics of UML (industry standard language) to assist business process description and profit consequent from the improvements achieved by the high level vision. To show the benefits of this new language applied to this specific business we model the engineer and manufacturing activity processes using VDML.

Publicado em:

Proceedings of 5th IEEE International Conference on Industrial Informatics INDIN 2007, 23 a 27 Julho 2007, Vienna, Austria.

VCO –VEHICLE CORPORATE ONTOLOGY

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Integration of Information in enterprises is a nightmare due to the differences in software and hardware platforms and due to syntactic and semantic differences in the data sources schemas. To help solve this problem we will propose and define a specific ontology for automobile industry (VCO) based on OWL and a specific UML2 profile. This ontology will address the problems of (soft-and hardware) platform and syntactic heterogeneity, provide rules to defined domain ontology and support mappings between individual schemas.

Keywords: Ontology, UML, MDA, Language.

Publicado em:
*Proceedings of 2nd
Conferência Ibérica
de Sistemas e
Tecnologias de
Informação
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June 2007, Porto.*

IR-CASE TOOL

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Publicado em:
*Proceedings of IASTED
 International
 Conference on
 Software Engineering
 (SE 2007), February 13
 to February 15, 2007,
 em Innsbruck, Austria.*

We propose a new approach based on a methodology assisted by a IR-Case tool for the creation of IR (Information Retrieval) systems inspired on a set of best practices or principles: it is based on high-level models or specifications; it is component-based architecture centric; it is based on generative programming techniques. This approach follows in essence the MDA (Model Driven Architecture) philosophy with some specific characteristics. We propose a repository that keeps related information, such as models, applications, software architectures, generated artifacts and even information concerning the software process itself (e.g., generation steps, tests and integration milestones). Generically, this methodology receives system requirements (e.g., functional, non-functional and development requirements) as its main input, and produces a set of artifacts (e.g., source code, configuration scripts or data scripts) as its main output, that will be linked in the IR-Case tool proposed, generating the IR-System. These aspects are implemented in a tool (IR-Case tool), providing a roadmap where designers can follow as well as model-to-model transformation templates in order to accelerate their system development tasks. This step facilitates the construction and consequently will contribute for the personalized IR-Systems and also a test platform for IR-Algorithms and IR-Process.

Keywords: UML, MDA, Retrieval Information, Case Tool.

A METHODOLOGY TO DESIGN INFORMATION RETRIEVAL SYSTEMS (MDIRS)

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MDIRS is methodology to define the actors and the steps to build efficiently information retrieval (IR) System. MDRIS main mission is to analyze, develop and evaluate mechanisms and tools to produce IR systems from a more abstract, high level, efficient and productive way than it is done currently. MDIRS project is influenced by MDA reference model, and is mainly based on three principles: namely, high-level models specification; generative programming techniques; and it is component-based architecture-centric. In this paper we detail the methodology generative programming techniques used to produce IR Systems and the work that will be handled in the near future.

Publicado em:
Proceedings of EATIS 2007, Euro American Conference on Telematics and Information Systems, 14-17 of May 2007, Algarve, Portugal.

A SCALABLE AND FLEXIBLE WEB SERVICES AUTHENTICATION MODEL

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*Proceedings of the
2007 ACM workshop
on Secure Web
Services, Fairfax, USA,
2 de Novembro de
2007, pp. 66-72.*

The WS-* specification set defines a message authentication model for web services. This model targets the authentication of message exchanges in large scale decentralized systems, composed by different authentication domains. However, it has scalability and flexibility limitations: the acquirement of identity claims requires online interactions with security token services, which introduces communication overhead and creates performance bottlenecks; the services' policies, containing its requirements, must directly point to the issuing security token services, limiting the flexibility of the trust relations.

We present a new model, addressing these limitations, using two concepts from the trust management paradigm: credentials for claim inference and claim-based issuer references (attribute based delegation). We show how credentials are used both to increase the scalability, reducing the number of online token requests, and to increase the flexibility by allowing indirect trust relations, namely claim based delegation. We also show how the simultaneous usage of security tokens and credentials results in several advantages of our model, when compared to credential only trust management models. The proposed model fits nicely into the WS-* framework, namely into its message security model and policy language. We illustrate this with the implementation of an extension to the Windows Communication Foundation - a commercial grade web services platform - that provides support for this model.

SISTEMA GLOBAL DE NAVEGAÇÃO POR SATÉLITE: PRINCÍPIOS, APLICAÇÕES E DESAFIOS

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A União Europeia está a criar um sistema mundial de navegação por satélite, formado pelo Galileo e pelo Egnos. Os benefícios desta tecnologia ficaram já demonstrados com o GPS dos EUA. São criadas continuamente aplicações que abrangem todas as actividades e todos os sectores da economia mundial e prevê-se que o mercado de produtos e serviços atinja 400 000 milhões de euros em 2025. Nesta comunicação abordam-se os princípios de funcionamento dos sistemas de navegação por satélite e dos sistemas complementares. Caracterizam-se os serviços de localização, navegação e cronometria, descreve-se a infra-estrutura e perspectiva-se a evolução tecnológica dos sistemas de navegação por satélite. Identificam-se domínios de aplicação, designadamente: serviços e chamadas de emergência assentes na localização; transporte rodoviário; transporte ferroviário; transporte marítimo e fluvial e pescas; aviação; protecção civil, gestão de situações de emergência e auxílio humanitário; mercadorias perigosas; transporte de animais; agricultura, medição de parcelas, geodesia e levantamentos cadastrais; energia, petróleo e gás; busca e salvamento; outras aplicações. Pretende-se contribuir para o aparecimento de ideias inovadoras sobre a utilização das tecnologias e serviços de navegação por satélite.

Publicado em:

*Semana Informática
2007, 6-8 de Março,
2007, Lisboa,
Portugal.*

IMPROVING PSEUDORANGE ESTIMATION IN GNSS RECEIVERS WITH A RECURSIVE BAYESIAN APPROACH

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Publicado em:
*Proceedings of the 6th
Conference on
Telecommunications,
Conftel 2007,
May 9-11, 2007,
Peniche, Portugal.*

A Global Navigation Satellite System (GNSS) receiver provides essentially two independent measurements of pseudorange through the estimation of code delay and carrier phase. Although the code delay estimate is an absolute (unambiguous) measurement its accuracy is hindered by noise; on the contrary, the phase estimate has, in general, better accuracy but is ambiguous. The Hatch filter has been used as the conventional solution to merge the two kinds of measurements. Herein, we propose an alternative solution based on the joint code delay/phase estimation using a bank of stochastic nonlinear filters. The phase ambiguity is progressively reduced by merging the code delay estimates with the phase estimates provided by the selected nonlinear filter.

ASYMMETRICAL STROBE PULSES FOR MULTIPATH MITIGATION IN BOC GNSS RECEIVERS

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Binary offset carrier (BOC) modulations have been proposed for new Global Navigation Satellite System (GNSS) signals, since they achieve better tracking performance than phase-shift keying in the presence of channel noise and multipath. Besides, the concept of delay lock-loop based on strobe pulses can be extended to BOC modulations with significant advantage in the close-in multipath region. Herein, a design technique of asymmetrical strobe pulses for BOC receivers is proposed and analyzed. A target code discriminator response with desirable characteristics is defined allowing to determine the strobe pulse as the solution of an integral equation. The resulting pulse provides good multipath mitigation capability, extended code tracking range, and lack of false code-lock points.

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Conference on
Telecommunications,
Conftele 2007,
May 9-11, 2007,
Peniche, Portugal.*

NONLINEAR LEAST-SQUARES ALGORITHM FOR CLOSE-IN MULTIPATH MITIGATION IN GNSS RECEIVERS

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Publicado em:
*Proceedings of the
ION GNSS 2007,
September 25-28,
2007, Fort Worth,
Texas.*

Multipath is one of the major sources of positioning errors in Global Navigation Satellite System (GNSS) receivers. In many cases, its effects are completely unpredictable and cannot be mitigated by differential reception techniques. Many different signal processing techniques have been proposed to minimize the multipath problem with different degrees of success depending on the excess delay between the direct path and the secondary path(s) of the satellite incoming signal. In general, they fail to solve the problem for very short excess delays (typically $\leq 0.1T_c$, where T_c stands for the code chip duration). However, it is for this range of delays (close-in region) that the distortion suffered by the direct ray may be stronger. It has been demonstrated that there is room for significant improvement in the performance of the multipath mitigation algorithms operating in the close-in region if alternative approaches to the conventional multipath mitigation techniques are considered. Herein, we propose a technique for close-in multipath minimization based on the Levenberg-Marquardt algorithm. Given a vector of parameters a that contains the delays of the line-of-sight and the reflected ray that hit the GNSS receiver and a set of observations, which depend nonlinearly on a , the Levenberg-Marquardt algorithm determines an iterative best-fit solution to a . Although the algorithm is computationally demanding it is feasible with today's signal processing technology for the usual update rates of the navigation equation (in the order of one Hz).

STOCHASTIC NONLINEAR FILTERING FOR ENHANCED PSEUDORANGE ESTIMATION IN GALILEO/GPS RECEIVERS

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Position evaluation using a Global Navigation Satellite System (GNSS) receiver requires, at least, the measurement of 4 satellite signal delays (pseudoranges). Two different types of measurements can be performed: the code delay and the carrier phase. The code delay measurements yield unambiguous but noisy pseudorange estimates. On the contrary, the estimates provided by the carrier phase are essentially noiseless although they are affected by an ambiguity term which is multiple of the carrier wavelength. The Hatch filter has been used as the standard solution to merge the two types of measurements. Herein, we propose an alternative solution based on the joint code delay/carrier phase estimation using a bank of stochastic nonlinear filters. The pseudorange ambiguity is progressively reduced by merging the code delay estimates with the phase estimates provided by the selected nonlinear filter.

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*Proceedings of the
URSI 2007
Symposium.*

CODEVOTING: PROTECTION AGAINST AUTOMATIC VOTE MANIPULATION IN AN UNCONTROLLED ENVIRONMENT

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Publicado em:

Actas da Conferência Internacional VOTE-ID 2007, Bochum, Alemanha, 4 a 5 de Outubro de 2007, Springer-Verlag LNCS 4896, pp. 178-188.

One of the major problems that prevent the widespread of Internet voting is the vulnerability of the voter's computer. A computer connected to the Internet is exposed to virus, worms, spyware, malware and other threats that can endanger the election's integrity. For instance, it is possible to write a virus that changes the voter's vote to one predetermined vote on election's day. It is possible to write such a virus so that the voter would not notice anything wrong with the voting application.

This attack is very dangerous because it may pass undetected. To prevent such attack it is necessary to prevent automatic vote manipulation at voter's computer. Here we present CodeVoting, a technique to create a secure communication channel to a smart card that prevents vote manipulation by the voter's PC, while at the same time allows the use of any cryptographic voting protocol to protect the election's integrity at the server side of the voting application.

Keywords: Internet voting, vote manipulation.

BOOSTING OF (VERY) WEAK CLASSIFIERS

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In this paper we apply boosting to weak (binary) learners. The main idea is to combine the output of several simple learners in order to obtain a better classifier. As weak learners we consider generative classifiers and radial basis function classifiers. Our tests on synthetic data show that the proposed algorithm has good convergence properties. On benchmark data, boosting of these weak learners attains results close to the well-known Real AdaBoost algorithm (with decision trees) and support vector machines, constituting a low complexity competitive choice.

Publicado em:

*Actas da 6th
Conference on
Telecommunications,
Peniche, Portugal,
9 a 11 de Maio de
2007.*

LONG DISTANCE REAL-TIME ECHO CANCELLATION

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Publicado em:
*Actas da 6th
Conference on
Telecommunications,
Peniche, Portugal,
9 a 11 de Maio de
2007.*

This paper describes an implementation of a long distance echo canceller, operating on full-duplex with hands-free and in real-time with a single Digital Signal Processor. The proposed solution is based on short length adaptive filters centered on the positions of the most significant echoes, which are tracked by time delay estimators. To deal with double talking situations a speech detector is employed. The floating-point DSP TMS320C6713 from Texas Instruments is used with software written on the C++ programming language using some compiler optimizations to reduce execution time. The resulting algorithm enables long distance echo cancellation with low computational requirements. It reaches greater echo return, loss enhancement and shows fast convergence speed than the conventional solution. Our experimental results also approach the CCITT G.165 recommendation.

CLUSTERING OF SCATTERERS IN MOBILE RADIO CHANNELS – AN APPROACH FOR MACRO-CELL ENVIRONMENT OVER IRREGULAR TERRAIN

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In this paper a realistic model that is an extension of COST 273 channel model, introducing terrain and clutter information into cluster generation, is presented. Our model is based on a geometrical/stochastic approach, and allows a realistic treatment of both cluster positions and dynamics. This is done by means of visibility regions. Using terrain and clutter information, the cluster and visibility region generating PDFs were derived. Some simulation results over a GIS tool for the city of Lisbon are presented.

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*6th IEEE Conference on
Telecommunications
2007, Peniche,
Portugal, 9-11 de Maio
de 2007.*

PERFORMANCE ENHANCEMENT USING MIMO TECHNIQUES FOR UMTS FDD

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In this paper Multiple Input Multiple Output (MIMO) techniques for Universal Mobile Telecommunication System (UMTS) analysis is presented. To simulate the radio channel the COST 259 directional channel model (DCM) is used for macro and microcell scenarios, as defined by the Third Generation Partnership Project (3GPP). Values of capacity and Bit Error Rate (BER) are obtained for different MIMO configurations. A capacity enhancement is achieved using MIMO with UMTS but different results for the BER metric were observed when a uniform power distribution is used through the antenna element array (AEA).

Publicado em:

*6th IEEE Conference on
Telecommunications
2007, Peniche,
Portugal, 9-11 de Maio
de 2007.*

CLUSTERING OF SCATTERERS OVER AN IRREGULAR CLUTTER ENVIRONMENT: AN EXTENSION OF COST 273 MIMO CHANNEL MODEL

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In this paper an extension of COST 273 channel model, introducing terrain and building information into cluster and visibility region generation, is presented. Using terrain and clutter information, the cluster and visibility region PDFs are derived and compared with previous results. Some simulation results for the city of Lisbon, Portugal, are presented.

Publicado em:

66th IEEE Vehicular Technology Conference Fall 2007, Baltimore, EUA, 30 de Setembro a 3 de Outubro de 2007.

A DYNAMIC PROPAGATION PREDICTION PLATFORM OVER IRREGULAR TERRAIN AND BUILDINGS FOR WIRELESS COMMUNICATIONS

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The paper introduces an algorithm that converts dynamically GIS terrain and clutter information into the flat terrain input parameterization needed for COST 231 Walfisch-Ikegami model. Under this algorithm, a new method for average building height calculation is presented, using Epstein-Peterson's multiple knife-edge diffraction method. Additionally, it is introduced a new realistic approach for line-of-sight stochastic modeling. The Mobile Station (MS) paths are generated using a new mobility model previously validated for the city of Lisbon, Portugal.

Publicado em:

66th IEEE Vehicular
Technology Conference
Fall 2007, Baltimore,
EUA, 30 de Setembro
a 3 de Outubro de
2007.

TERRAIN AND CLUTTER IMPACT ON JOINT STATISTICAL PROPERTIES OF AZIMUTH SPREAD AND DELAY SPREAD IN MACRO-CELL BAD URBAN ENVIRONMENT

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In this paper a realistic directional channel model that is an extension of COST 273 channel model is presented. The model uses a previously developed cluster and visibility generation strategy with increased realism, due to the introduction of terrain and clutter information. The new model was implemented in Matlab using terrain, clutter, street and user mobility information for the city of Lisbon, Portugal. The simulation analysis was performed and joint statistical properties of azimuth spread and delay spread were compared with other models and available experimental data. The introduction of clutter and terrain information into the simulations produces an increase on multi-path delay and azimuth spread, underlining Lisbon's bad urban characteristics.

Publicado em:

IEEE International Symposium on Wireless Communication Systems 2007, Trondheim, Norway, 17-19 October 2007.

AN IMPROVED DIRECTIONAL CHANNEL MODEL OVER IRREGULAR TERRAIN AND CLUTTER

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In this paper, new improvements and results for a previously developed directional channel model are presented. The directional channel model is an extension of COST 273 channel model, introducing terrain and building information into radio channel simulation. New approaches for path-loss prediction and Line of Sight (LoS) modeling are considered, affecting the cluster path gain model implementation. The complete radio channel model was implemented using terrain, clutter, street and user mobility information for the city of Lisbon, Portugal. Some of the model's outputs are presented, mainly path loss and small/large-scale fading statistics.

Publicado em:

10th International Symposium of Wireless Personal Multimedia Communications 2007, Jaipur, India, Dezembro de 2007, (IS).

UMA FERRAMENTA PARA CÁLCULO DE COBERTURA RÁDIO EM TÚNEIS RODOVIÁRIOS - APLICAÇÃO AO TÚNEL DO CORTADO, MADEIRA

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O presente artigo apresenta o estudo para cobertura rádio a 108 MHz de um túnel rodoviário, utilizando como área de projecto o maior túnel do país: o Túnel do Cortado, na Região Autónoma da Madeira (3200m). São apresentados os modelos de cobertura indoor estudados e adaptados a este projecto, bem como os passos necessários para a criação de uma aplicação em MatLab que permitiu simular a cobertura rádio. A ferramenta desenvolvida funciona de forma modular permitindo escolher: modelo utilizado, tipo de antena, localização e direcção da antena, frequência e potência de emissão. Após o desenvolvimento da aplicação foi possível implementar uma solução optimizada que garantiu cobertura em 97% da área.

Publicado em:

1.º Seminário do
Comité Português da
URSI

"Radiocomunicações -
Novos paradigmas e
impacto na saúde",
Novembro de 2007.

MAXIMIZAÇÃO DE DESEMPENHO SOBRE ENHANCED UMTS USANDO A TECNOLOGIA HSDPA

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1.º Seminário do
Comité Português da
URSI

"Radiocomunicações -
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impacto na saúde",
Novembro de 2007.

No presente artigo é analisado o desempenho de uma ligação típica da tecnologia *Universal Mobile Telecommunications System* (UMTS) associada aos sistemas de telecomunicações móveis de terceira geração (3G), utilizando modulação adaptativa introduzida pela tecnologia *High Speed Downlink Packet Access* (HSDPA). Esta técnica consiste em escolher, para cada trama de bits transmitida, a modulação mais adequada às condições do canal. Os aspectos básicos do problema são formulados analiticamente considerando a transmissão com modulações PSK (*Phase Shift Keying*) e QAM (*Quadrature Amplitude Modulation*) num canal com desvanecimento e efeito *Doppler*. Para considerar um modelo mais realista, foi desenvolvido um programa de simulação capaz de modelar o sistema considerando os principais componentes do sistema HSDPA, padronizado para transmissão de dados em alta velocidade na ligação descendente. O desempenho da ligação foi avaliado para diversas situações através da taxa de erro de bit, da taxa de transmissão média e do *throughput* obtido na transmissão, procurando-se investigar a influência de parâmetros do sistema nesse desempenho.

AN ADAPTIVE DOMAIN KNOWLEDGE MANAGER FOR DIALOGUE SYSTEMS

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This paper describes the recent effort to improve our Domain Knowledge Manager (DKM) that is part of a mixed-initiative task based Spoken Dialogue System (SDS) architecture, namely to interact within an ambient intelligence scenario. Machine-learning applied to SDS dialogue management strategy design is a growing research area. Training of such strategies can be done using human users or using corpora of human computer dialogue. However, the size of the state space grows exponentially according to the state variables taken into account, making the task of learning dialogue strategies for large-scale SDS very difficult. To address that problem, we propose a divide to conquer approach, assuming that practical dialogue and domain-independent hypothesis are true. In this context, we have considered a clear separation between linguistic dependent and domain dependent knowledge, which allows reducing the complexity of SDS typical components, specially the Dialoguer Manager (DM). Our contribution enables domain portability issues, proposing an adaptive DKM to simplify DM's clarification dialogs. DKM learns, through trial-and-error, from the interaction with DM suggesting a set of best task-device pairs to accomplish a request and watching the user's confirmation. This adaptive DKM has been tested in our domain simulator.

Publicado em:

*9th International
Conference on
Enterprise Information
Systems, 2007, 45-52.*

ADAPTAÇÃO DE UM SISTEMA DE DIÁLOGO AO DOMÍNIO BILHÉTICA

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This paper describes our research in order to adapt a Dialogue System (DS) to a ticket-selling domain. We have considered a task based DS architecture, which interacts within an Ambient Intelligence (Aml) scenario with a set of knowledge-based artifacts. Each artifact has its own knowledge model, linked to lexical resources, defining a semantic interface. In this paper, we propose the reuse of the Aml domain model in the ticket-selling domain redefining the abstractions of artifact, class, and task.

Publicado em:

5th Workshop in Information and Human Language Technology, 2007, 1733-1736.

ABSTRACTION LEVEL REGULATION OF COGNITIVE PROCESSING THROUGH EMOTION-BASED ATTENTION MECHANISMS

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In domains where time and resources are limited, the ability to balance resource consumption according to the problem characteristics and to the required solution quality is a crucial aspect of intelligent behavior. Growing evidence indicates that emotional phenomena may play an important role in that balance. To support this view we propose an agent model where emotion and reasoning are conceived as two symbiotically integrated aspects of cognitive processing. In this paper we concretize this view by extending emotion-based regulation of cognitive activity to enable an active control of the abstraction level at which cognitive processes operate through emotion-based attention mechanisms, thus allowing a dynamical adjustment of the resources used. Experimental results are presented to illustrate the proposed approach and to evaluate its effectiveness in a scenario where reasoning under time-limited conditions in a dynamic environment is required.

Publicado em:

Proceedings of the 4th International Workshop on Attention in Cognitive Systems – 20th International Joint Conference on Artificial Intelligence, Hyderabad, India, 6 - 12 de Janeiro de 2007, pp. 7-20.

A SIGNAL BASED APPROACH TO ARTIFICIAL AGENT MODELING

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In this paper we propose an approach to agent modelling that follows a signal based metaphor where agents are modelled as dissipative structures and their cognitive structures are modelled as compositions of multiple energetic potentials. This uniform representational support is used to model both reactive and deliberative processes. To illustrate the descriptive adequacy of the model, two experimental cases are presented where reactive and deliberative processes are modelled based on the proposed approach.

MODELING THE DYNAMIC NONLINEAR NATURE OF EMOTIONAL PHENOMENA

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The study of emotional phenomena, particularly the development of emotion models for intelligent agent implementation has been mainly based on a perspective of emotion as a human phenomenon. In this paper we present an alternative view where emotional phenomena are neither rooted on cognitive nor on nervous structures, but on bio-physical principles that are pervasive among biological organisms. A primary contribution of this paper is to show how it is possible to explain in a single unified framework the existence of identifiable emotional patterns and, at the same time, the continuous nonlinear nature of emotion processes.

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Second International
Conference on
Affective Computing
and Intelligent
Interaction, Lisboa,
Portugal, 12 - 14 de
Setembro de 2007,
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OPTICAL ABSORPTION AND APPARENT BANDGAP OF ACETYLENE-BASED DLC FILMS

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28 de Maio a 1 de
Junho de 2007.*

Diamond-like carbon (DLC) films can be deposited at higher deposition rates when acetylene C_2H_2 is used instead of the commonly employed CH_4 source gas. However, film quality may suffer as far as optical absorption and transport properties are concerned. We have decomposed a mixture of acetylene and hydrogen by conventional plasma CVD at 13.54MHz at low substrate temperature up to 400°C. Indeed, with acetylene alone the deposition rate reached values as high as 80nm per minute. Films from pure acetylene showed a yellowish colour consistent with appreciable optical absorption in the 400 to 700nm range. Broad Urbach tails were obtained from the absorption spectra. For example, with hydrogen dilution at 98% the deposition rate dropped by a factor of 10, on the other hand the transparency improved substantially. On selected films we measured the photo and dark conductivity. Films were further analysed by infrared absorption spectra between 400 and 4500 cm^{-1} . To estimate the relative amount of graphitic material the individual contributions of sp^3-CH , $sp^3-CH_{2,3}$ and sp^2 species were determined from the individual peak intensities at 2850, 2920, and 2950 cm^{-1} , respectively. We are investigating further improvements of film quality by increasing plasma power and hydrogen dilution to reduce remaining graphitic components.

ANALYSIS AND SIMULATION OF A-SI:H/A-SiC:H PINIP STRUCTURES FOR COLOR IMAGE DETECTION

Fantoni, A.; Martins, J.; Fernandes, M.; Louro, P.; Vieira, M.

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It is presented in this paper a study on the photo-electronic properties of multilayer a-Si:H/a-SiC:H p-i-n-i-p structures. This study is aimed to give an insight into the internal electrical characteristics of such a structure in thermal equilibrium, under applied bias and under different illumination condition. Taking advantage of this insight it is possible to establish a relation among the electrical behavior of the structure, the structure geometry (*i.e.* thickness of the light absorbing intrinsic layers and of the internal n-layer) and the optical properties of the layers (*i.e.* optical bandgap controlled through the percentage of carbon dilution in the a-Si_{1-x}C_x:H layers).

Behaving as a phototransistor, showing optical gain for low incident light power at a variety of wavelength peak response controllable by means of externally applied bias or structure composition, these structures are quite attractive for photo-sensing device applications, like color sensors and large area color image detector.

An analysis based on a theoretical model, a SPICE simulation of an equivalent electrical model and a numerical ASCA simulation are executed for describing the behavior of different configurations of the device and compared with experimental measurement about spectral response and current-tension characteristic. Finally it is presented a conclusion about the applicability of these devices in large area electronic applications.

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SPECTRAL RESPONSE CHARACTERIZATION OF A-SI:H-BASED MIS-TYPE PHOTODETECTORS

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 Junho de 2007.*

Amorphous silicon (a-Si:H) PIN photodiode and MIS photoelectric converter are two alternative sensing elements used in indirect-conversion flat panel X-ray detectors. The major advantage of the MIS structure over PIN is that the photosensor and the TFT switch can be fabricated simultaneously resulting in effective reduction in the lithography mask count. However, the noise level and sensitivity of the MIS-type photosensor are strongly dependent on the properties of the dielectric-semiconductor interface, which should be controlled for successful device fabrication. In this paper we describe a method and a test setup developed to measure the transient dark current and spectral response characteristics of the a-Si:H MIS photosensors. Since the dynamic range of the sensor is limited, the spectral characterisation was performed using lock-in technique under very low intensity of non-modulated light. The digital averaging technique was used to measure a dark current decay in a wide time domain. Using this novel method the segmented gate/SiNx/(i)a-Si:H/(n+)a-Si:H /ITO structures have been characterized under different biasing conditions. The test results along with a device model are presented and discussed. It is found that the amplitude of the time-dependent component of the leakage current induced by defects at the SiNx/a-Si:H interface can be significantly reduced by adjusting the biasing conditions. The observed changes in the spectral response characteristics with variations of the refresh pulse amplitude are easily understood by analyzing the charge carrier transport in the active layer under different wavelengths of the incident light.

SPIN POLARIZATION OF DILUTED MAGNETIC SEMICONDUCTORS UNDER THE IMPURITY PHOTOEXCITATION

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One of the most efficient methods to control and manipulate spin polarization in diluted magnetic semiconductors (DMS) is controllable illumination with polarized light. There is currently a need to develop a theory to explain existing experimental data, taking into the account the long-time relaxation (LTR) mechanisms. In this paper we propose a system of kinetic equations which describe dynamics of the non-equilibrium spin systems of band electrons and electrons occupying the impurity levels. It is assumed that the semiconductor is illuminated with the polarized light of frequency corresponding to the impurity absorption. The presence of LTR processes is taken into account for band electrons and magnetic ions, together with the processes of thermal impurity ionization and spin-spin interaction of the band and impurity electrons. We present analytical expressions to determine the spin polarization degrees of band electrons h_e through the spin polarization h_s of magnetic ions. The stationary space-inhomogeneous distributions of spin-polarized electron concentrations and polarization degrees h_e and h_s are studied numerically as a function of the polarization type (clockwise, counter-clockwise, linear) and intensity of light, magnitude of the LTR times, etc. We calculated the dynamics of the spin subsystem using parameters typical of InP:Fe. It is shown that the distribution of electron concentration in thick films shows damped oscillations, the amplitude of which coincides with the stationary space-homogeneous distribution on the back side of the sample (opposite to the illuminated side). The concentration of spin-polarized band electrons is by more than four orders of magnitude larger than the intrinsic carrier concentration. The linear-polarized light enhances the concentration of the band electrons three times due to the transitions between the impurity level and conduction band; counter-clockwise polarized light allows to obtain two-times higher concentrations, while the clockwise polarized light enhances the concentration only by 150%. The results are in good agreement with existing experiments.

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Junho de 2007.*

INDIUM OXIDE THIN-FILM TRANSISTOR BY REACTIVE ION BEAM ASSISTED DEPOSITION

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This work reports on the fabrication and characterization of indium oxide semiconducting films and their application in thin-film transistors (TFTs). The films have been deposited at room temperature by oxygen ion beam assisted e-beam evaporation. The influence of deposition conditions on film properties including the crystal structure, conductivity, stoichiometry, and intrinsic stress is analyzed. It is found that the electrical properties of indium oxide films can be engineered from metallic to insulating and the film structure can be varied from amorphous to microcrystalline by adjusting evaporation rate, oxygen ion energy, and ion beam flux. Furthermore, the highly-resistive films with considerable microstructural crystallinity exhibit n-type field-effect behaviour. A field-effect mobility of $1.4\text{cm}^2/\text{V}\cdot\text{s}$, and current on-to-off ratio of 10^6 are observed for transistors with a silicon dioxide gate dielectric.

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de Electrónica da
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de 2007.*

SPECTRAL RESPONSE ANALYSIS OF A-SiC:H PINIP PHOTODIODES

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ISEL - Electronics Telecommunication and Computer Dept., Lisboa, Portugal

We present in this paper results about the analysis of photocurrent and spectral response in a-SiC:H/a-Si:H pinpin and pinip structures. Our experiments and analysis reveal the photocurrent profile to have a strong nonlinear dependence on the externally applied bias and on the light absorption profile, *i.e.* on the incident light wavelength and intensity. Our interpretation points out the cause of such effect to a self biasing of the junctions under certain unbalanced light generation of carriers and to an asymmetric reaction of the internal electric fields to the externally imposed bias. The possibility to relate such a behavior to the light intensity and wavelength indicates realistic hypothesis of using these structures and this effect for color recognition sensors. We present results about the experimental characterization of the structures and numerical simulations obtained with the program ASCA. Considerations about electrical field profiles and inversion layers will be taken into account to explain the optical and voltage bias dependence of the spectral response. Our results show that in both structures the application of an external electrical bias (forward or reverse) mainly influences the field distribution within the less photo excited sub-cell.

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MULTISPECTRAL STRUCTURES FOR IMAGING APPLICATIONS

Vieira, M.; Fantoni, A.; Fernandes, M.; Louro, P.

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 International SENSOR
 COMM 2007, Valência,
 Espanha, de 14 a 19
 de Outubro de 2007.*

In this paper we present results on the optimization of an $\text{pin}^2\text{i}^2\text{n}$ type a-Si:H based three color detector with voltage controlled spectral sensitivity. The sensor element consists of a glass/ITO/p-i-n a-SiC:H multilayer structure which faces the incident illumination, followed by $\text{a-SiC:H}(-\text{p})/\text{a-SiC:H}(-\text{i})/\text{Si:H}(-\text{i}')/\text{SiC:H}(-\text{n}')/\text{ITO}$ heterostructure, that allows the optically addressed readout. Results show that this approach leads to regionally different collection parameters resulting in multispectral photodiodes, coding for red (R), blue (B), and two green (G) components. In the polychromatic operation mode different sensitivity ranges are selected by switching between different biases so that the basic colors can be resolved with a single device. Positive bias is needed under blue irradiation and moderated reverse bias under green. The threshold voltage between green and red sensitivity depends on the thickness of the bottom $\text{a-SiC:H}(-\text{i})$ layer, and corresponds to the complete confinement of the absorbed green photons across the $\text{pin}^2\text{i}^2\text{n}$ sequence. As the thickness of the $\text{a-Si:H}(-\text{i}')$ layer increases, the self-reverse effect due to the front absorption will be balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias. The various design parameters are discussed and supported by a 2D numerical simulation.

LASER SCANNED MODULATED BARRIER PHOTODIODE: AN ELECTRICAL MODEL

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The devices analyzed in this work present an S-shape J-V characteristic when illuminated. By changing the light flux a non linear dependence of the photocurrent with illumination is observed. Thus a low intensity light beam can be used to probe the local illumination conditions, since a relationship exists between the probe beam photo-current and the steady state illumination. Numerical simulation studies showed that the origin of this S-shape lies in a reduced electric field across the intrinsic region, which causes an increase in the recombination losses. Based on this, we present a model for the device consisting of a modulated barrier recombination junction in addition to the p-i-n junction. The simulated results are in good agreement with the experimental data.

Using the presented model a good estimative of the LSP signal under different illumination conditions can be obtained, thus simplifying the development of applications using the LSP as an image sensor, with advantages over the existing imaging systems in the large area sensor fields with the low cost associated to the amorphous silicon technology.

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OPTICAL IMAGE AND COLOR RECOGNITION USING MONOLITHIC TANDEM PINIP AND PINPIN HETEROJUNCTIONS: A COMPARISON

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de Outubro de 2007.*

Optimized a-SiC:H multilayer devices based on two different tandem configurations (TCO/pinpi'n/TCO and TCO/pini'p/TCO) are compared and tested for proper image recognition and color separation process using an optical readout technique. In both configurations the doped layers are based on a-SiC:H to increase image resolution and to prevent image blurring. To profit from the light filtering properties of the active absorbers, the intrinsic layer of the front diode (i layer) is based on a-SiC:H and the back one (i' layer) on a-Si:H.

The effect of the applied voltage on the color selectivity is discussed. Results show that the relative spectral response curves demonstrate rather good separation between the red, green and blue basic colors. Combining the information obtained under positive and negative applied bias a colour image is acquired, using the same optical technique either in pinpi'n or in the pini'p configuration, without colour filters or pixel architecture.

PINPI'N AND PINPII'N MULTILAYER DEVICES WITH VOLTAGE CONTROLLED OPTICAL READOUT

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Louro, P.¹; Lavareda, G.^{2,3}; Carvalho, C.N.^{2,3}**

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In this paper we present results on the optimization of a pinpii'n type a-Si:H based three color detector with voltage controlled spectral sensitivity. The sensor element consists on a glass/ITO/p-i-n a-SiC:H multilayer structure which faces the incident illumination, followed by a-SiC:H(-p)/a-SiC:H(-i)/Si:H(-i')/SiC:H (-n)/ITO heterostructure, that allows the optically addressed readout.

Results show that this approach leads to regionally different collection parameters resulting in multispectral photodiodes, coding for red (R), blue (B), and two green (G) components. In the polychromatic operation mode different sensitivity ranges are selected by switching between different biases so that the basic colors can be resolved with a single device. Positive bias is needed under blue irradiation and moderate reverse bias under green. The threshold voltage between green and red sensitivity depends on the thickness of the bottom a-SiC:H (-i) layer, and corresponds to the complete confinement of the absorbed green photons across the pinpi sequence. As the thickness of the a-Si:H i'-layer increases, the self-reverse effect due to the front absorption will be balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias. The various design parameters are discussed and supported by a numerical simulation.

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MODELING A-SiC:H TANDEM PINPIN AND PINIP PHOTODIODES FOR COLOR SENSOR APPLICATION

Fantoni, A.; Martins, J.; Fernandes, M.; Louro, P.; Vygranenko, Y.; Vieira, M.

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Lisboa, Portugal

The present paper reports the optical properties of multilayer structures composed by p-i-n cells based on a-SiC:H or a-Si:H material. Different structures are studied in order to obtain image sensors that accomplish color filtering in addition to image pattern recognition. A simple theoretical model is developed to explain sensors behavior and to derive the optical-readout experimental procedure. Electrical models for the sensors are established for simulation purposes and to compare photocurrent signals with experimental data. A numerical simulation of the JV characteristic and of the spectral response is also presented in order to show possible future optimization of the device. Two main structures are studied, namely p-i-n/p-i-n and p-i-n/n-i-p tandem cells.

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15 de Janeiro de 2007.*

AMORPHOUS HYDROGENATED CARBON FILMS DEPOSITED FROM ACETYLENE

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Diamond-like carbon (DLC) films can be deposited at higher deposition rates when acetylene C_2H_2 is used instead of the commonly employed CH_4 source gas. However, film quality may suffer as far as optical absorption and transport properties are concerned. We have decomposed a mixture of acetylene and hydrogen by conventional plasma CVD at 13.54MHz at low substrate temperature up to 400°C. Indeed, with acetylene alone the deposition rate reached values as high as 100nm per minute. Films from pure acetylene showed a yellowish colour consistent with appreciable optical absorption in the 400 to 700nm range. Broad Urbach tails were obtained from the absorption spectra. For example, with hydrogen dilution at 98% the deposition rate dropped by a factor of 10, on the other hand the transparency improved substantially. On selected films we measured the photo and dark conductivity. Films were further analysed by infrared absorption spectra between 400 and 4500 cm^{-1} . To estimate the relative amount of graphitic material the individual contributions of sp^3 -CH, sp^3 - $CH_{2,3}$ and sp^2 species were determined from the individual peak intensities at 2850, 2920, and 2950 cm^{-1} , respectively. We are investigating further improvements of film quality by increasing plasma power and hydrogen dilution to reduce remaining graphitic components.

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NON LINEAR EFFECTS IN THE PHOTOCURRENT BEHAVIOUR: A REQUIREMENT IN THE LASER SCANNED PHOTODIODE TECHNIQUE

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Publicado em:
Livros de Resumos da Conferência International Meeting on Development in Materials, Processes and Applications of Nanotechnology, Belfast, Reino Unido, 15 de Janeiro de 2007.

The Laser Scanned Photodiode (LSP) concept enables the fabrication of large area image sensors with application in fields where low cost, and design simplicity are of major importance. The LSP technique relies on the fact that the photocurrent of the device does not change linearly with the light intensity, and thus the local illumination conditions over the active area of the structure can be evaluated by measuring the current generated by a low power light beam. The device is a large area p-i-n amorphous silicon based structure deposited over a glass substrate by a PECVD technique with two semitransparent electrical contacts. In order to decrease the conductivity of the doped layers methane is introduced in the reactor during the growth of the n and p layers. This step is of major importance since the lateral currents in the doped layers degrade the sensor performance.

AMORPHOUS CARBON FILMS GROWN BY CVD USING ACETYLENE SOURCE GAS

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Diamond-like carbon (DLC) and CVD diamond films are usually prepared by microwave plasma using highly hydrogen-diluted methane as source gas. A general handicap is the low deposition rate. Other carbon-containing source gases showed much larger growth rates. However, film quality may suffer as far as optical absorption and transport properties are concerned.

In a comparative study J. Robertson has shown that both benzene and acetylene are attractive alternatives for methane. We have decomposed a mixture of acetylene and hydrogen by conventional plasma CVD at 13.54MHz at low substrate temperature up to 400°. Indeed, with acetylene alone the deposition rate reached values of 80nm per second. This can be compared with the deposition rate for silane CVD under similar process conditions of only about 2nm/s. Films from pure acetylene showed a yellowish colour consistent with appreciable optical absorption in the 500 to 700nm range. Increasing the hydrogen dilution to 98% brought the deposition rate down by a factor of 8, however, it improved the transparency substantially. From the absorption spectra we deduced band gap values of 2 to 3 eV, depending on process pressure and substrate temperature. Films on glass started to peel rapidly, whereas adhesion was perfect on crystalline silicon. On the other hand, analysis of the curvature and size of detached hillocks allowed us to calculate internal tensile stress.

Films were further analyzed by infrared absorption spectra between 400 and 4500cm⁻¹. To estimate the relative amount of graphitic material the respective sp³ and sp² contributions of C-Hn species with individual peaks at 2860 and 2930cm⁻¹, respectively, were analyzed. A peak at 2350cm⁻¹ is correlated to the broad signal at 3050cm⁻¹, both increase strongly with increasing hydrogen dilution.

Another criterium for film quality is the ratio between light and dark conductivity which we measured in the visible until the near UV region. The broad below band gap defect distributions, as evidenced by wide Urbach tails, improved with increasing hydrogen dilution. We are investigating further improvement of film quality by increasing plasma power, substrate temperature, and hydrogen dilution to reduce graphitic components.

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STRUCTURE OF DIAMOND-LIKE CARBON FROM ACETYLENE

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Tetrahedral amorphous carbon (ta-C) or diamond-like carbon (DLC) films can be deposited at higher deposition rates when acetylene or acetylene + hydrogen mixtures are used instead of the commonly employed CH₄ source gas. However, film quality may suffer as far as optical absorption and transport properties are concerned. We have decomposed the mixture by conventional plasma CVD at 13.54MHz at low substrate temperature up to 400°C.

The films have been prepared using a wide range of power, temperature and dilution conditions. The composition and optical properties of the DLC films have been characterized by UV spectroscopy and Fourier transform infrared spectroscopy (FTIR).

Indeed, with acetylene alone the deposition rate reached values as high as 80Å per minute. Broad Urbach tails were obtained from the absorption spectra. For example, with hydrogen dilution at 90% the deposition rate dropped by a factor of 10, on the other hand the transparency improved substantially. The great versatility of carbon materials arises from the strong dependence of the ratio of sp² and sp³ bounds in the material. Films were further analysed by infrared absorption spectra between 400 and 4500cm⁻¹. To estimate the relative amount of graphitic material the individual contributions of sp³-CH, sp³-CH_{2,3} and sp²-CH₂ species were determined from the individual peak intensities at 2850, 2920, and 3035 cm⁻¹, respectively.. With high H₂ dilution a very intense peak appears in the 2250-2350cm⁻¹ region, which can be related to a triple bond between two carbon atoms. Mass spectrometry data will presented with the aim to study the correlation between plasma species and film properties.

A-SiC:H MULTILAYER STRUCTURES: AN ELECTRICAL SIMULATION BASED ON SPICE MODELS

Martins, J.; Louro, P.; Fernandes, M.; Vieira, M.

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The present paper reports the optical properties of multilayer structures composed by p-i-n cells based on a-SiC:H or a-Si:H material. Different structures are studied in order to obtain image sensors that accomplish color filtering in addition to image pattern recognition. A theoretical model consistent with well known semiconductor equations is established to explain sensors behavior and to derive the optical-readout experimental procedure. Electrical models for the sensors are established for simulation purposes and to compare photocurrent signals with experimental data. Two main structures are studied, namely p-i-n/p-i-n and p-i-n/n-i-p tandem cells.

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OPTICAL CONTROLLED SPECTRAL SELECTIVITY IN MULTILAYER HETEROSTRUCTURES

**Vieira, M.¹; Louro, P.¹; Fantoni, A.¹;
Fernandes, M.¹; Lavareda, G.^{2,3}; Carvalho, C.N.^{2,3};**

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19 a 22 de Março de
2007.*

Large area hydrogenated amorphous silicon single and stacked p-i-n structures with low conductivity doped layers are proposed as monochrome and color image sensors. The layers of the structures are based on amorphous silicon alloys (a-Si_xC_{1-x}:H). The current-voltage characteristics and the spectral sensitivity under different bias conditions are analyzed. The output characteristics are evaluated under different read-out voltages and scanner wavelengths. To extract information on image shape, intensity and color, a modulated light beam scans the sensor active area at three appropriate bias voltages and the photoresponse in each scanning position (“sub-pixel”) is recorded. The investigation of the sensor output under different scanner wavelengths and varying electrical bias reveals that the response can be tuned, thus enabling color separation. The operation of the sensor is exemplified and supported by a numerical simulation.

TWO TERMINAL OPTICALLY ADDRESSED COLOUR AND IMAGE PROCESSING DEVICE

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A two terminal optically addressed colour and image processing device based on two stacked sensing/switching p-i-n a-SiC:H diodes is presented. The charge packets are optically injected into the p-i-n sensing photodiode and confined at the illuminated regions changing locally the electrical field profile across the p-i-n switching diode. A red scanner is used for charge readout.

The various design parameters and addressing architecture tradeoffs are discussed. The influence on the sensor output characteristics of the a-SiC:H/a-Si:H absorber thickness optimized for red transmittance and blue and green collection is analysed. Results show that the thin a-SiC:H sensing absorber confines the readout to the switching diode and light filters the structure allowing full colour detection at two appropriated voltages. A physical model supports the image and colour recognition process.

Publicado em:

Livros de Resumos da Conferência Fourth IEEE International Conference on Smart Systems and Devices, Hammamet, Tunísia, 19 a 22 de Março de 2007.

IMAGING APPLICATIONS USING MULTISPECTRAL STRUCTURES AND AN OPTICAL READOUT

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Publicado em:
*Livros de Resumos da
Conferência Fourth
IEEE International
Conference on Smart
Systems and Devices,
Hammamet, Tunísia,
19 a 22 de Março
de 2007.*

In this paper we present results on the optimization of an pinpin type a-Si:H based three color detector with voltage controlled spectral sensitivity. The sensor element consists of a glass/ITO/p-i-n a-SiC:H multilayer structure which faces the incident illumination, followed by a-SiC:H(-p)/a-SiC:H(-i)/Si:H(-i')/SiC:H(-n')/ITO heterostructure, that allows the optically addressed readout. Results show that this approach leads to regionally different collection parameters resulting in multispectral photodiodes, coding for red (R), blue (B), and two green (G) components. In the polychromatic operation mode different sensitivity ranges are selected by switching between different biases so that the basic colors can be resolved with a single device. Positive bias is needed under blue irradiation and moderated reverse bias under green. The threshold voltage between green and red sensitivity depends on the thickness of the bottom a-SiC:H (-i) layer, and corresponds to the complete confinement of the absorbed green photons across the pinpin sequence. As the thickness of the a-Si:H i'-layer increases, the self-reverse effect due to the front absorption will be balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias. The various design parameters are discussed and supported by a 2D numerical simulation.

LOW-AREA, LOW-POWER PARALLEL ADCs OBTAINED BY USING LOW-PRECISION COMPARATORS

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Full-parallel ADCs are used with high sampling rates and low/medium resolution. The number of comparators is doubled for each additional bit in resolution. However, the cost should be measured by area and power consumption, rather than by the number of circuit elements. In this paper we use comparators with very low area and low power, which have high offset voltage; using Wallace-tree encoding is equivalent to performing comparator reordering, and the resolution is improved without using offset compensation or calibration. This technique is demonstrated by statistical simulation. As an example, we designed a 6 bit ADC in a $0.18\mu\text{m}$ CMOS technology, with 0.4mm^2 area and power consumption of 5mW at 200MSamples/s . A figure-of-merit of 0.5 pJ /conversion is obtained.

Publicado em:

XXII Conference on Design of Circuits and Integrated Systems - DCIS 2007, Sevilha, 21 a 23 de Novembro de 2007.

PRICING EXOTIC DERIVATIVES ON INTEREST RATE PRODUCTS: SOME PRACTICAL ISSUES

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We present some methodologies used to create pricing instruments of exotic derivatives on interest rate products. We underline the main issues encountered in the process as well as the techniques used to overcome these issues.

Publicado em:

*Livro de Resumos de
International
Conference on
Advances in
Interdisciplinary
Statistics
and Combinatorics,
Univ. of North Carolina
at Greensboro,
Greensboro,
North Carolina, USA,
12 a 14 de Outubro
de 2007.*

OPTION PRICING WITH GAUSSIAN PROCESSES

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Models based on Gaussian Processes have become commonplace for problems of regression and classification in the machine learning community. One key aspect in using Gaussian Processes for machine learning is to have enough prior information on the data in order to specify mean and covariance functions.

Under the Black-Scholes model for pricing options, the options underlying log returns follows a normal distribution with known mean and covariance functions. In this article we present a machine learning approach to options pricing under the Black-Scholes model, based on Gaussian Processes.

We model the log returns of the options underlying with a Gaussian Process, in order to estimate the volatility, and then model the options prices with another Gaussian Process. We use a constant mean function for the log returns of the underlying and the Black-Scholes options price closed form formula as the options prices mean function. In both cases we use a squared exponential covariance function as the Gaussian Processes kernel. We compare option prices computed by the Gaussian Process model with the prices computed with the common closed form Black-Scholes formula, using synthetic data.

This machine learning approach to options pricing as the advantage of providing a measure of confidence of volatility and prices, which is a valuable indicator of how well the model is representing the data over time.

Publicado em:

Livro de Resumos de XLI Euro Working Group on Financial Modelling, Lisboa, Portugal, 8 a 10 de Novembro de 2007.

A CEPSTRUM-BASED METHOD FOR REMOTE TRAIN DETECTION

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Publicado em:

*Proceedings of the
Fourteenth
International Congress
on Sound and
Vibration (ICSV14),
09-12 July 2007,
Cairns, Australia.*

On the subject of remote train detection, previous work has already been made, applying different techniques. The system described in this paper, comprises both hardware (receiver circuit connected to an accelerometer) and software subsystems. The latter subsystem employs a technique based on vector quantization (VQ). Through a training process, two centroids have been derived, resulting from the application of an unsupervised learning algorithm (Lloyd algorithm), using a 20th-order Cepstral analysis. Each centroid represents one of two different classes of signals: “Silence” (or absence of a moving train) and “Moving train” (approaching or withdrawing). What is being presently proposed is an alternative to a previous representation of the centroids, in which they were derived from a 14th-order Linear Predictive Coding (LPC) analysis. Similarly, incoming signals coming from the receiver must also undergo a Cepstral analysis. The input of the software subsystem consists of samples of the input signal, obtained by the hardware subsystem. Sampling rate is 16,000 samples per second, being the samples windowed into 300ms frames, with a window displacement of 100ms. The recognition (or classification) process is based on a distance measure to each one of the two centroids. The Euclidean vector distance measure was used for this purpose. Collected data was divided into training and classification corpora, respectively 67% and 33%. There were considered situations in which one had trains running on the same track where the receiver is connected to, and trains running on neighbour tracks, being the vibrations transmitted through the ground to the receiver circuit. For both situations, classification results are presented and discussed, comparing performances between the Cepstrum-based and the LPC-based pattern matching processes.

TOWARDS AUTOMATED VERIFICATION OF WEB SERVICES

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This paper proposes the use of model-checking software technology for the verification of workflows and business processes behaviour based on Web services, namely the use of the SPIN model checker. Since the specification of business process behaviour can be decomposed into patterns, it is proposed a translation of a well known collection of workflow patterns into PROMELA, the input specification language of SPIN. The use of this translation is illustrated with one business process example, which demonstrates how its translation to a PROMELA model can be useful in the Web service specification and verification.

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IADIS WWW/Internet
2007, Oct. 2007.

A SIMILARITY MEASURE FOR MUSIC SIGNALS

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Publicado em:
*Proceeding of the 10th
International
Conference on
Interprise Information
Systems, Barcelon,
Spain, 12-16, June
2008.*

One of the goals in the field of Music Information Retrieval is to obtain a measure of similarity between two musical recordings. Such a measure is at the core of automatic classification, query, and retrieval systems, which have become a necessity due to the ever increasing availability and size of musical databases. This paper proposes a method for calculating a similarity distance between two music signals. The method extracts a set of features from the audio recordings, models the features, and determines the distance between models. While further work is needed, preliminary results show that the proposed method has the potential to be used as a similarity measure for musical signals.

4.2V TOLERANT BUCK CONVERTER IN A STANDARD 3.3V 0.13 μ m CMOS TECHNOLOGY

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In this paper the design of integrated buck converters, tolerant to supply voltages higher than the process limit for individual CMOS transistors, is presented. In particular, the topologies for the level shifters and the power block are analyzed. Different driving solutions for a general circuit topology that use cascoded transistors in the output stage and can tolerate nearly twice the process voltage limit are discussed. A buck converter core incorporating an optimized usage of this power block and a modified version of a conventional voltage shifter was designed in a standard 3.3V, 0.13 μ m CMOS process. The converter is powered by a lithium-ion battery with a voltage range from 2.7V to 4.2V, and can deliver an output current up to 100mA with a programmable output voltage from 0.6V to 2.0V, with up to 90% efficiency. A methodology is presented for verification of high voltage compatibility of circuits design using low voltage technologies.

Publicado em:

Proc. International Conference on Power Engineering, Energy and Electrical Drives, POWERENG 2007, April 12-14 2007, Setúbal, Portugal.

HIGH VOLTAGE TOLERANT LEVEL SHIFTERS AND LOGIC GATES IN STANDARD LOW VOLTAGE CMOS TECHNOLOGIES

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- 2 Dept. de Eng. Electrotécnica e de Computadores, IST, Lisboa, Portugal
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- 5 Chipidea Microelectronics, Lisboa, Portugal

In this paper, high voltage (HV) tolerant level shifters with combinational functionality are proposed based on Differential Cascode Voltage Switch Logic (DCVSL). These level shifters are tolerant to supply voltages higher than the process limit for individual CMOS transistors. The proposed HV DCVSL level shifters are particularly useful when it is mandatory to ensure a specific behavior during out of the normal mode periods (power up; power down; reset; etc.). These high voltage tolerant logic circuits were used in the power block of a buck converter designed in a standard 3.3V, 0.13 μ m CMOS process, powered by an input voltage range from 2.7V to 4.2V.

Publicado em:

*Proc. 6th Conference on
Telecommunications –
ConfTele 2007,
May 9-11 2007,
Peniche, Portugal.*

HIGH VOLTAGE TOLERANT LEVEL SHIFTERS AND DCVSL IN STANDARD LOW VOLTAGE CMOS TECHNOLOGIES

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Costa, J. Dores^{3,4}; Lima, Floriberto⁵**

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In this paper, high voltage (HV) tolerant level shifters with combinational functionality are proposed based on Differential Cascode Voltage Switch Logic (DCVSL). These level shifters are tolerant to supply voltages higher than the process limit for individual CMOS transistors. The proposed HV DCVSL level shifters are particularly useful when it is mandatory to ensure a specific behavior during out of the normal mode periods (power up; power down; reset; etc.). These high voltage tolerant logic circuits were used in the power block of buck converter designed in a standard 3.3V, 0.13 μ m CMOS process, powered by an input voltage range from 2.7V to 4.2V.

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*Proc. IEEE
International
Symposium on
Industrial Electronics
(ISIE 2007), June 4-7
2007, Vigo, Spain.*

OPTIMIZATION OF OBSERVATION TIME FOR OBTAINING THE PROFILE OF MUSCULAR LOAD USING THE APDF FUNCTION

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Electromyographic signals (EMG) may be used to analyze the muscular strain during work. The Amplitude Probability Distribution Function (APDF) provides a statistical quantitative measure of muscle activity for a period of time. The established recording time to properly estimate this distribution function is one hour of recording. This paper presents a systematic analysis, based on real EMG data, of the period of time necessary to estimate the profile of the muscular load during the period of work using the APDF function. It is shown that it is possible to estimate this function based on a reduced period of time quantifying the uncertainty of the estimate.

Publicado em:

*Actas da ConfTele
2007 (6th Conference
on Telecommunications),
Peniche, Maio de
2007.*

ESTIMATION OF THE ACQUISITION TIME FOR OBTAINING THE PROFILE OF MUSCULAR LOAD USING THE APDF FUNCTION

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The Amplitude Probability Distribution Function (APDF) of an EMG signal provides a statistical measure of the variation of load on muscles. In vocational studies it is suggested a typical recording time of one hour. The aim of our study is to prove that it is possible to reduce the acquisition window to estimate the profile of muscular load using the APDF.

Publicado em:

Actas da PREMUS 2007 (Sixth International Scientific Conference on Prevention of Work-Related Musculoskeletal Disorders), Boston, 27-30 August 2007.

STRING PATTERNS: FROM SINGLE CLUSTERING TO ENSEMBLE METHODS AND VALIDATION

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Publicado em:

*Actas da 7th
International
Workshop on Pattern
Recognition in
Information Systems
PRIS-2007, Funchal,
Junho de 2007.*

We address the problem of clustering of string patterns, in an Ensemble Methods perspective. In this approach different partitioning of the data are combined attempting to find a better and more robust partition. In this study we cover the different phases of this approach: from the generation of the partitions, the clustering ensemble, to the combination and validation of the combined result. For the generation we address, both different clustering algorithms (using both the hierarchical agglomerative concept and partitional approaches) and different similarity measures (string matching, structural resemblance). The focus of the paper is the concept of validation/selection of the final data partition. For that, an information-theoretic measure in conjunction with a variance analysis using bootstrapping is used to quantitatively measure the consistency between partitions and combined results and choose the best obtained result without the use of additional information. Experimental results on a real data set (contour images), show that this approach can be used to unsupervisedly choose the best partition amongst alternative solutions, as validated by measuring the consistency with the ground truth information.

INTERLIGAÇÃO DE DOMÍNIOS SIP – O ESTUDO DOS PROBLEMAS E SUAS SOLUÇÕES

Cruz, Nuno Miguel Machado

Mestrado em: Engenharia Electrotécnica e Computadores

Grau Concedido por: Instituto Superior Técnico

Orientadores: Mário Serafim Nunes

Provas Concluídas em: 20 de Junho de 2007

Esta dissertação propõe uma arquitectura que permite implementar uma infra-estrutura VoIP baseada em SIP com capacidade de interligação a outras infra-estruturas existentes. A arquitectura proposta é baseada em componentes *open source* e assenta no princípio de ser a menos intrusiva possível na rede, coexistindo assim com mecanismos de NAT e *firewalls*. Ao mesmo tempo pretende disponibilizar o máximo de controlo à equipa de gestão da rede. A arquitectura proposta foi obtida após diferentes testes aos componentes disponíveis no mercado e foi inclusive colocada em produção numa das instituições de teste. Os resultados obtidos demonstram a compatibilidade elevada da arquitectura proposta com os componentes existentes. Demonstra ainda que o objectivo foi cumprido, permitindo assim a interligação genérica de diferentes instituições através de VoIP.

INTEGRAÇÃO DINÂMICA DE ARTEFACTOS EM SISTEMAS DE DIÁLOGO

Borges, Luís Ricardo

Doutoramento em: Informática e Computadores

Grau Concedido por: Universidade Técnica de Lisboa

Orientadores: Nuno João Neves Mamede e Manuel Martins Barata

Provas Concluídas em: 23 de Março de 2007

A modelação de aplicações de língua natural que permitem às pessoas conversarem com máquinas/computadores, da mesma forma que conversam entre si, é materializada sob a forma de um sistema de diálogo, constituindo uma interface natural, onde o uso da fala é privilegiado. Esta dissertação descreve um processo, ao nível do conhecimento, que permite a integração dinâmica de artefactos no domínio de aplicação de um sistema de diálogo. Neste cenário, considera-se que o domínio do sistema de diálogo é constituído por um conjunto de artefactos heterogêneos, com cardinalidade variável em tempo de execução. Estes artefactos, dispersos num ambiente inteligente, rodeiam os utilizadores na sua vida quotidiana. Cada artefacto é visto como um recurso computacional cuja gestão é atribuída, em tempo de execução, ao sistema de diálogo. O processo de integração bilateral proposto permite de forma robusta balancear e agilizar estratégias de concepção dos sistemas de diálogo, flexibilizando a sua concepção e adaptação ao domínio de aplicação. Atendendo a que a modelação de conhecimento tem custos significativos, este trabalho também é uma contribuição para reduzir os custos de desenvolvimento e de manutenção dos actuais sistemas de diálogo.

SEGUIMENTO DE PESSOAS E GRUPOS EM SINAIS DE VÍDEO COM REDES BAYESIANAS

Jorge, Pedro Miguel Torres Mendes

Doutoramento em: Engenharia Electrotécnica e de Computadores

Grau Concedido por: Instituto Superior Técnico

Orientadores: Prof. Jorge dos Santos Salvador Marques e

Prof. Arnaldo Joaquim de Castro Abrantes

Provas Concluídas em: 26 de Março de 2007

Esta dissertação apresenta um algoritmo para o seguimento de pessoas em sequências de vídeo, capaz de lidar com oclusões. As oclusões podem ser causadas por elementos estáticos da cena ou devido à formação de grupos de pessoas. Pretende-se que o sistema recupere o seguimento das pessoas em movimento assim que deixem de estar ocluídas.

É proposto um algoritmo com dois níveis. O primeiro nível produz um conjunto de segmentos de trajectória das pessoas em movimento, a partir da sequência de vídeo, enquanto estas estão visíveis. Estes segmentos obtêm-se por associação de regiões activas detectadas em imagens consecutivas. Sempre que há oclusões, há uma interrupção na associação de regiões e são criados novos segmentos. Para ultrapassar esta dificuldade, o segundo nível realiza uma etiquetagem (*labeling*) consistente dos segmentos de trajectória utilizando um modelo estatístico baseado em redes bayesianas. Os segmentos de trajectória que recebem a mesma etiqueta devem corresponder à trajectória de uma única pessoa. A rede bayesiana é construída dinamicamente ao longo da sequência de vídeo e serve de base para o cálculo da interpretação (etiquetas) mais provável, utilizando os dados extraídos até esse instante. Cada vez que é recolhida nova informação, as trajectórias são reclassificadas, o que permite a recuperação de erros recentes. São apresentados testes experimentais para ilustrar o desempenho do algoritmo em situações complexas.

COLOUR AND IMAGE SENSORS WITH ADDRESSED OPTICAL READOUT

Antunes, Paula Maria Garcia Louro

Doutoramento em: Eng.^a Electrotécnica

Grau Concedido por: Universidade Nova de Lisboa

Orientadores: Adolfo Steiger Garção e Maria Manuela Vieira

Provas Concluídas em: 2 de Outubro de 2007

O objectivo principal desta tese de doutoramento consiste em desenvolver e otimizar sensores de imagem e de cor com leitura e endereçamento ópticos.

Procedeu-se primeiramente à caracterização estrutural e optoelectrónica dos filmes finos semicondutores baseados em silício amorfo hidrogenado (a-Si:H) e ligas de siliceto de carbono (a-SiC:H) que constituem os dispositivos sensores.

Os sensores foram analisados em estrutura simples e empilhada. Realizou-se a análise das suas características de saída através de medições de corrente-tensão (I-V) em regime dc e ac; de capacitância-tensão (C-V) e de resposta espectral sob diversas condições de polarização luminosa e eléctrica. Os princípios de funcionamento físico foram explicados através da simulação numérica dos perfis de potencial, de campo eléctrico e das taxas de geração e de recombinação de portadores.

Nos dispositivos de estrutura simples o estudo realizado visou essencialmente otimizar a resistividade das camadas dopadas para melhorar o desempenho do sensor no que respeita a resolução, gama dinâmica, linearidade, selectividade espectral, etc.. Analisou-se igualmente um sensor p-i-n em substrato flexível para aplicações biométricas. Da análise da configuração simples concluiu-se que o acoplamento óptico entre o processo de leitura e de escrita induz uma baixa relação sinal-ruído, e que a selectividade na absorção de luz visível é igualmente baixa.

Por este motivo configurações empilhadas baseadas em homo e/ou heteroestruturas p-i-n de a-Si:H foram analisadas. A utilização de uma grelha metálica entre os elementos de escrita e de leitura é igualmente discutida. Estas configurações permitem melhorar a qualidade da imagem obtida através da técnica de leitura óptica mas revelam-se incapazes de reconhecer as três cores fundamentais. Para ultrapassar esta limitação analisaram-se outras configurações empilhadas em que a camada intrínseca do fotodiodo de leitura se baseia num semicondutor de maior hiato óptico (a-SiC:H), o que melhora não só a absorção da luz de baixos comprimentos de onda como também a

transparência à luz de maiores comprimentos de onda. Nestas circunstâncias os dispositivos p-i-n-p-i-n foram otimizados de modo a separar convenientemente a absorção das três cores base do sistema de representação de cor RGB. Com o dispositivo otimizado foram reconstruídas imagens a cores usando um algoritmo de baixo nível.



03

ENGENHARIA MECÂNICA

Anuário Científico 2007

ISEL

A DESIGN APPROACH TO FDI/FTC OF COMPLEX NETWORKED CONTROL SYSTEMS

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The design of fault tolerant control (FTC) systems of large-scale complex networked control systems (NCS) is a difficult task due to the large number of sensors and actuators spatially distributed and networked connected. Despite the research effort on developing FTC systems most of these developments are designed globally leading to centralized FTC solutions inadequate to NCS. In this paper we present the first version of a toolbox based on multi-agent systems to design FTC systems for large-scale complex NCS. This toolbox is based on a decentralized FTC of NCS which relies on causal graph partitioning of the NCS digraph model and on intelligent distributed computing using multi-agents systems.

Publicado em:

*Journal of Control
Engineering and
Applied Informatics,
2007, Vol. 9, n. 4,
3-11.*

“POSTPONEMENT” IN THE LOGISTICAL SYSTEMS OF NEW AUTOMOBILES MARKETING IN PORTUGAL: THE BRANDS AND QUALITY

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Publicado em:

Total Quality Management, 2007, Vol. 18, n. 6, 681-696.

Automobile production is a worldwide industry in which quality has always been a very prominent and pertinent issue. There exists, however, certain links in the logistical chain that involve local initiatives in the finishing of the final product – including final testing, repairs to breakdowns and damage that occurred during transport operations. There also exists a group of steps or links in this type of operation, designated as “postponement”, including delicate tasks of customization which, if they are not well carried out, may bring into question the integrity of the vehicle, its future reliability and the image of the make or brand. These are therefore of no minor importance in the overall issue. In the case of Portugal we find that it is the transporters who secure the distribution process from gate release at the production line through to delivery to the final customer, as indicated by the local concessionaire. This long logistical segment includes the above-mentioned postponement operations, carried out at appropriate logistical platforms or support facilities. It may be considered rather surprising therefore to discover that quality certification of these platforms or supports is not a priority objective for the automobile manufacturers, for their concessionaires or even the final customer, a situation quite the opposite to that which occurs in the factories themselves on their vehicle or component production lines. Finally, strategic logistics formulation emerges like a strategy foundation supported in logistics competencies; from logistics strategy to strategic logistics.

A FUZZY CONTROLLER FOR A HEALTH SERVICES MOBILE ROBOT

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The purpose of this paper is to present the devolvement of a fuzzy control applied for hospitals and health care centers mobile concept robot, the i-MERC. The robot and fuzzy controller models are presented as well as simulation results. The simulation application that was developed included the possibility to change de bending radius of the curves. To analyze the performance of the robot in following curves posing different dynamic demands simulations were performed considering curves with an abrupt change of direction and with 10, 20, 30, 40 and 50cm of radius. A virtual reality resource allows demonstrating the service concept with the purpose of searching stakeholders interested in the project.

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In Proceedings of IEEE 2007, the 2007 IEEE International Symposium on Industrial Electronics, Vigo, Spain, 4-7 June 2007, pp. 3287- 3292.

HYBRID FAULT DETECTION AND ISOLATION IN A HEATER BANK OF AN HVAC SYSTEM

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 and Automation,
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 T14-009.*

Heating, Ventilation and Air-Conditioning (HVAC) systems are widely used in different environments. Current HVAC systems are complex and integrate different control schemes, instruments, mechanical components, etc. Operating twenty four hours a day, these systems have to keep the quality and temperature of air in buildings, to maintain the comfort of the occupants. The performance of the control system should ideally be good even in the presence of a fault, to avoid causing discomfort in the building occupants. FDI and FTCS are methodologies that can be applied to HVAC systems to make them as robust as possible to potential faults. The application of FDI methods to HVAC systems has been proposed using different methods. Because HVAC systems are highly nonlinear and complex systems, different strategies to solve particular problems can be investigated. In this paper, a methodology is presented for fault detection and isolation using multiple models. A hybrid technique that includes probabilistic and optimization based methods is presented. The method is applied, both in simulation and by means of real-time experiments, to the heating unit of a Heating, Ventilation Air Conditioning (HVAC) system. It is shown that the addition of the probabilistic approach improves the fault diagnosis accuracy.

RISK MANAGEMENT BASED ON A CRITICALITY CENTRED MAINTENANCE METHODOLOGY (CCM)

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In this work a methodology for risk management is presented based on the maintenance performed on critical components during the systems life cycle and taking in account the operational environment where those systems are at work. To know the critical values for each component a multidisciplinary team work is needed. The criteria to quantify the relative criticality of each component to the process when it fails include several important parameters, such as economic losses, environment consequences and the safety of workers. A risk management is put on work, focusing the maintenance efforts on those which show the unacceptable values, so reducing their criticality to acceptable values. This is a dynamic process which requires periodic review of input parameters.

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Livro de Proceedings da ESREL2007 – European Safety and Reliability Conference, Stavanger, Norway, 25-27 June 2007, pp. 313-318.

GLOBAL VALUE CHAINS – ICT AS COMPETITIVE ADVANTAGE

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Working Conference
on Virtual Enterprises,
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Nowadays, the cooperative intelligent transport systems are part of a largest system; transportations are modal operations integrated in logistics; and, logistics is the main process of the supply chain management. The supply chain strategic management as a simultaneous local and global (“glocal”) value chain is a collaborative/cooperative organization of stakeholders, many times in co-opetition, to perform a service to the customers respecting the time, place, price and quality levels. The transportation, like other logistics operations must add value, which is achieved in this case through compression lead-times and order fulfilments.

The aim of this paper is evidence and proposes the use of Radio Frequency Identification (RFID) technologies integrated into an Information and Communication Technologies (ICT) framework based on Distributed Artificial Intelligence (DAI) supported by a Multi-agent system (MAS) approach, as the most value advantage of Supply Chain Management (SCM) in a cooperative intelligent logistics systems.

MAINTENANCE OF FIRE PROTECTION EQUIPMENTS AND FIRE RISK ASSESSMENT

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As there is a greater concern about the safety of critical industries all over the world, fire risk plays an important role because in the majority of the cases this event can result in catastrophic consequences for life, equipments and continuity of activities or even environmental hazard. Fire protection equipments with low reliability means that these equipments are often unavailable and thus the risk of fire consequences increases. Maintenance plays an important role in this issue. These kinds of systems are most time in a dormant mode, which gives uncertainty about the functionality and operability when demanded in a real situation of fire. This paper outlines the importance of tests, inspection and maintenance operations in this context and proposes a methodology based in international standards and supported in reports to correct the frequency of these actions according to the real state of degradation of components and safety purposes.

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Livro de Proceedings da RQR2007 – Risk, Quality and Reliability - International Conference, Ostrava, Czech Republic, 20 and 21 September 2007, pp. 159-168.

MULTI-AGENT PLATFORM FOR FAULT TOLERANT CONTROL SYSTEMS

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International
Conference on
Systems, Man and
Cybernetics
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Canadá, 7-10 de
Outubro de 2007,
pp. 1321-1326.*

This paper proposes a new multi-agent platform for Fault Tolerant Control (FTC) Systems. Several multi-agent platforms exist to deal with different problems but none of them to deal with control systems tolerant to faults using the Matlab/Simulink® environment, which is in our days the scientific bench to this kind of research. When dealing with large-scale complex networked control systems (NCS), designing FTC systems is a very difficult task due to the large number of sensors and actuators spatially distributed and network connected. To solve this issue, the FTC platform presented in this paper uses simple and verifiable principles coming mainly from a decentralized design based on causal modelling partitioning of the NCS and distributed computing using multi-agent systems paradigm, allowing the use of agents with well established FTC methodologies or new ones developed taking into account the NCS specificities.

SEGURANÇA INDUSTRIAL E DO TRABALHO NO CONTEXTO INTERNACIONAL: “SEVESO” E “PIC”

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As preocupações, ao nível da segurança industrial, com os efeitos em Estados terceiros, tanto na saúde humana (trabalhadores e populações) como no ambiente, encontram-se vertidas, ao mais alto nível, em instrumentos multilaterais internacionais da Organização das Nações Unidas.

Constituem exemplos paradigmáticos desta acção internacional concertada a Convenção ETAI - Efeitos Transfronteiriços de Acidentes Industriais Graves - da Comissão Económica para a Europa das Nações Unidas e a Convenção PIC - Procedimento de Prévia Informação e Consentimento - da Organização das Nações Unidas.

Em ambos os casos a Comunidade Europeia tem sido precursora: se por um lado a Convenção ETAI radica como matriz inspiradora e referencial na Directiva Seveso, por outro os industriais comunitários encontravam-se já obrigados ao disposto na Convenção PIC antes da sua entrada em vigor, indo-se mesmo mais longe nas obrigações impostas aos agentes económicos.

Efectua-se nesta comunicação uma introdução aos instrumentos internacionais em apreço.

Refere-se a legislação comunitária pertinente – Directiva 96/82/CE e Regulamento (CE) 304/2003 – seus pressupostos, objectivos e metodologias.

Com referência à regulamentação nacional de transposição – Decreto-Lei nº 254/2007 e Decreto-Lei nº 112/2007 – explicitam-se as obrigações (tanto de análise técnica como de gestão da segurança) que incumbem aos operadores envolvidos no fabrico, armazenagem e exportação, designadamente, no caso Seveso, Relatório de Segurança, Sistema de Gestão da Segurança, Plano de Emergência (interno e externo), Comunicação de Acidentes Graves e, no caso PIC, Notificação de Exportação, Consentimento Expresso.

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Actas do II Encontro Nacional de Riscos, Segurança e Fiabilidade - Riscos Públicos e Industriais, Secção Portuguesa da Associação Europeia de Segurança e Fiabilidade (ESRA), Lisboa, 13-15 de Novembro de 2007, volume 2, pp.86-882.

A IMPORTÂNCIA DA FIABILIDADE DOS EQUIPAMENTOS DE PROTECÇÃO CONTRA INCÊNDIO NA GESTÃO DO RISCO INDUSTRIAL

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Devido à enorme preocupação sobre o risco de incêndio, vários sectores industriais em todo o mundo encaram esta situação com grande preocupação. Na maioria dos casos este tipo de evento pode resultar em consequências catastróficas para a vida humana, equipamentos e continuidade das actividades ou até causar danos ambientais graves. Quando os equipamentos de protecção contra incêndio possuem baixa fiabilidade, tal significa que esses equipamentos estão frequentemente indisponíveis, aumentando o risco. Assim, torna-se importante que os estudos incidam sobre dois aspectos: a previsão da fiabilidade e a melhoria da fiabilidade. Este trabalho centra-se neste aspecto particular e pretende mostrar a importância da fiabilidade dos equipamentos de protecção contra incêndio num contexto de risco industrial. Neste tipo de sistemas podemos identificar o peso dos vários componentes de um ponto de vista fiabilístico, ou o seu impacto na fiabilidade do sistema, e actuar de acordo com os objectivos de segurança definidos. Assim, o trabalho realizado começa com uma introdução ao tema, passando depois pela definição de risco, sendo seguida de uma breve descrição sobre o risco particular de incêndio, onde se pretende mostrar a todos aqueles que ainda não estão consciencializados com a temática da segurança contra incêndios a sua importância, relatando factos relacionados com a sua probabilidade de ocorrência e com as suas consequências. Por fim, explica-se a importância da fiabilidade dos equipamentos de protecção contra incêndio e como se pode melhorar essa mesma fiabilidade. O artigo termina com um exemplo simples de cálculo e melhoria da fiabilidade, assim como algumas considerações finais sobre o trabalho apresentado.

VR STUDIO AS AN AUXILIARY TOOL FOR TECHNICAL EDUCATION

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The work presented in this paper promotes the use of Virtual Reality applications in teaching scenarios. Two applications are described which address different levels of knowledge acquisition and subject areas. Supporting these applications is VR Studio, a toolbox for Matlab which was developed as a rapid prototyping tool for Virtual Reality applications.

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*Actas do IEEE
Education Society
Engenharias'07, Univ.
Beira Interior, Covilhã,
21-23 Novembro
de 2007.*

DETECÇÃO DE DEFEITOS EM ROLAMENTOS – UMA APROXIMAÇÃO DIDÁCTICA

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*Actas da 4.^a
Conferência de
Engenharia
"Engenharia' 2007 -
Inovação e
Desenvolvimento",
IEEE Education
Society, Covilhã,
21 a 23 de Novembro
de 2007.*

As frequências de defeito de um rolamento são facilmente calculadas tendo em conta as velocidades relativas entre os vários elementos constituintes deste. No entanto, para se elaborar um diagnóstico eficaz, não se deve limitar a análise ao simples cálculo das frequências por aplicação directa das expressões matemáticas. O analista deve ter também presente a forma como o rolamento defeituoso gera essas frequências e os factores que permitem justificar a diferença entre as frequências teóricas calculadas e as medidas e emitidas pelo rolamento. Condensar a informação existente nesta área específica do Controlo de Condição e comparar os resultados dos vários ensaios realizados é o objectivo deste trabalho.

ANÁLISE E TRATAMENTO DE PARÂMETROS REAIS DE DEGRADAÇÃO NA ÓPTICA DA MANUTENÇÃO CONDICIONADA

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Sempre que seja possível prever a ocorrência de uma avaria pela deterioração do valor de algum parâmetro indicativo da condição de uma máquina ou sistema, e se isso puder ser feito com tempo suficiente para se poder planear uma intervenção, então estamos perante uma situação em que a manutenção condicionada ou preditiva é aplicável. Esta manutenção é realizada em função do estado dos componentes ou equipamento, sendo a intervenção efectuada apenas com a manifestação da necessidade. É uma manutenção preventiva, subordinada a um tipo de acontecimento predeterminado, como a informação de um sensor, a uma medida de um desgaste, ou outro indicador que possa revelar o estado de degradação do equipamento. É geralmente aplicada a máquinas vitais para a produção, a equipamentos cuja avaria compromete a segurança e a equipamentos críticos, com avarias caras e frequentes. Entre as técnicas usadas em manutenção condicionada, incluem-se: análise de vibrações, termografia, análise de óleos de lubrificação, análise de partículas, ferrografia, inspecção por ultra sons, inspecção radiográfica, etc. A manutenção condicionada não substitui integralmente os métodos mais tradicionais de manutenção correctiva e manutenção preventiva. No entanto, pode ser um complemento muito poderoso quando integrada num programa global de manutenção. No controlo de condição dos equipamentos um dos métodos aplicados é o acompanhamento da tendência, onde se procede à medição periódica ou contínua de um ou vários parâmetros indicadores da condição de funcionamento do equipamento. Com base nos valores medidos pode elaborar-se uma tendência que permite determinar quando a degradação da máquina atinge um valor crítico. O tempo que decorrerá até à ocorrência da avaria é a principal vantagem da utilização do sistema. A aplicação de estratégias de organização correctas, tal como o TPM e o RCM, só são verdadeiramente eficazes com a utilização de uma manutenção condicionada apoiada em modernos meios de controlo do estado de condição dos equipamentos e pelo conhecimento da evolução dos equipamentos e seus componentes ao longo do tempo. Através deste princípio, pretende-se neste artigo

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Nacional de
Manutenção,
Matosinhos,
22 a 23 de Novembro
de 2007.*

mostrar a importância do tratamento dos parâmetros reais recolhidos, aplicando uma metodologia, onde se pode estimar a tendência da falha e o momento em que a mesma potencialmente poderá ocorrer, sendo um método alternativo à estimativa do intervalo P(revention)-F(ailure), devido à dificuldade que por vezes existe na sua determinação. Exemplifica-se a aplicação da metodologia mostrando um caso prático real, com recurso a um programa informático.

ELECTROCHEMICAL BEHAVIOUR OF NITIT

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Near equiatomic nickel-titanium (Nitinol) is characterized by a unique combination of properties, including superelasticity and shape memory effect that makes it very attractive for biomedical applications, such as orthopaedic implants, self-expanding stents or orthodontics applications. Due to these properties, the material has the ability to return to a previously defined shape or size when subjected to an appropriate stress or thermal procedure, thus allowing a constant stress to be applied, e.g. for a more stable fixation of fractures.

The primary concern about Nitinol is the high nickel content and its possible influence on biocompatibility. In fact, nickel may generate allergenic, toxic and carcinogenic effects. On the other hand, conflicting views regarding the corrosion resistance of Nitinol, and therefore nickel ions release, have been found in the literature.

In the present work, the corrosion behaviour of NiTi in Hank's solution at 37°C was assessed by the use of electrochemical methods. Pure titanium and pure nickel were included in the study in order to understand the contribution of each alloying element. The results were compared with Ti 6Al 4V alloy and 316L stainless steel, materials traditionally used as orthopaedics implants. Moreover, the susceptibility of NiTi to corrosion under different conditions was examined using different physiological solutions and different pH values.

It was observed that the corrosion behaviour of NiTi is much closer to Ti than to Ni, as may be seen on the polarization curve results, where the high protective character of the passive oxide film formed on NiTi is similar to that of titanium. On the other hand, comparing the different implant materials it was possible to establish the following relation for their corrosion resistances: 316L stainless steel < NiTi < Ti-6Al-4V.

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do X Iberic Meeting
of Electrochemistry,
Coimbra, 12 a 14 de
Abril de 2007.*

ELECTRODEPOSITION OF POLYPYRROLE ON ALUMINUM ALLOY 6061-T6

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Electrochemistry,
Coimbra, 12 a 14 de
Abril de 2007.*

Due to their low cost, light weight and high mechanical resistance, aluminium alloys have been widely used in aerospace industry. In order to improve the corrosion resistance of these metals, different procedures can be adopted. Among them pre-treatments based on the use of chromates were widely investigated in the past. However, they have been classified as hazardous to environment and human health. Thus, much effort has been undergoing to develop new friendly and non-polluting coating systems.

Inherently conducting polymers (ICP) are attracting attention as possible components of corrosion-resistant coating systems in alternative to chromate-based treatments. These polymers can be deposited on the substrate by electropolymerization from a monomer solution. Among ICP's investigated for corrosion protection, polypyrrole is one of the most studied.

The present study reports the production of films of polypyrrole on aluminium alloy 6061-T6 by electropolymerization of pyrrole (0.5M) in a solution 0.5M H₂SO₄ and the assessment of their electrochemical behaviour. The electrodeposition was carried out by cyclic voltammetry or by potentiostatic methods. Electrochemical activity and corrosion protection properties of these films were investigated via dc polarization, electrochemical impedance spectroscopy and cyclic voltammetry. The morphology of the films was studied by scanning electron microscopy.

The results show that the polypyrrole films produced in aluminium alloy 6061-T6 are homogeneous and with a globular morphology but they don't confer significant corrosion protection to the metal.

A INTEGRAÇÃO DE FACTORES DE RISCO NA GESTÃO DE PROJECTOS INDUSTRIAIS MULTIDISCIPLINARES, COM RECURSO À DINÂMICA DE SISTEMAS

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Um projecto industrial caracteriza-se pela integração multidisciplinar de ciências de Engenharia e pela inerente complexidade decorrente da articulação e desenvolvimento de múltiplas actividades concorrentes.

Desta situação decorre com demasiada frequência a evidência de sobre custos, atrasos relativamente a datas-chave e deficiências ao nível da qualidade.

A integração da gestão de riscos na gestão do ciclo de vida de um projecto consubstancia-se como uma vertente essencial na contenção daquelas adversidades.

Logo que consolidada a Engenharia Processual, segue-se um conjunto de actividades associadas à engenharia de detalhe do projecto, que por antecederem fases de aquisição de materiais, de equipamentos e da construção, condicionam em grande medida o sucesso do Projecto.

O objectivo do presente artigo é o de analisar contribuição de diversos autores relativamente à identificação de factores de risco, a nível de engenharia de projecto de detalhe, propondo a sua integração na gestão do projecto através de modelos de dinâmica de sistemas, na expectativa de contribuir para a abertura de novos caminhos de investigação.

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Actas do II Encontro Nacional de Riscos, Segurança e Fiabilidade - Riscos Públicos e Industriais, Secção Portuguesa da Associação Europeia de Segurança e Fiabilidade (ESRA), Lisboa, 13-15 de Novembro de 2007, volume 1, pp.287-290.

ANÁLISE DE RISCOS NUMA EMPRESA DO SECTOR ELÉCTRICO E ELECTRÓNICO

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Actas do II Encontro Nacional de Riscos, Segurança e Fiabilidade - Riscos Públicos e Industriais, Secção Portuguesa da Associação Europeia de Segurança e Fiabilidade (ESRA), Lisboa, 13-15 de Novembro de 2007, volume 2, pp.1271-1286.

A apresentação de estudos de caso sobre iniciativas organizacionais em matéria de Segurança, Higiene e Saúde do Trabalho (SHST) incentiva as PME's a agir com iniciativas semelhantes e conduz, por isso, a uma melhoria das condições de segurança e saúde dos trabalhadores.

Nesta perspectiva apresenta-se um estudo de caso que se enquadra na necessidade de desenvolvimento de estudos na área de SHST, como um meio de incentivar os gestores a empreenderem acções e estratégias de cariz preventivo por forma a obterem benefícios em termos de mais valias e de competitividade reforçada.

O estudo teve por objectivo uma análise da segurança, do sector de produção de uma empresa do sector eléctrico e electrónico, em três fases: análise dos acidentes de trabalho; análise da cultura organizacional e de segurança e a análise de riscos.

Nesta comunicação apresenta-se a aplicação da metodologia da Matriz de Falhas à situação concreta.

Este método foi seleccionado após a análise dos acidentes de trabalho e a análise da cultura organizacional e de segurança da empresa, pois só neste enquadramento consideramos possível (a partir da metodologia de análise de riscos) apresentar medidas de resolução adequadas para as situações encontradas.

CONCEPÇÃO DE ROBÔS MÓVEIS APLICADOS AOS SERVIÇOS DE SAÚDE

Fonseca Carreira, Fernando Paulo Neves da

Mestrado em: Engenharia de Concepção

Grau Concedido por: Instituto Superior Técnico

Orientadores: Carlos Carreira e Arlindo Silva

Provas Concluídas em: 9 de Maio de 2007

O transporte de refeições nos serviços de saúde em condições de segurança e a transmissão eficiente de informações acerca das dietas personalizadas dos doentes são um desafio diário para todos os intervenientes no processo. A contaminação bacteriológica das refeições e da cozinha, os métodos utilizados para identificação das refeições demasiado arcaicos e ineficientes e a dificuldade em manipular os veículos quando estão carregados são os maiores problemas sentidos nos serviços de logística alimentar.

Para melhorar a qualidade dos serviços de entrega de refeições nos serviços de saúde, propõe-se um transportador automático – o i-Merc – – desenvolvido em duas versões, autónoma e servo-assistida, com compartimentos pré-aquecidos, um sistema de controlo da temperatura das refeições e um sistema de gestão de refeições integrado.

Na versão autónoma, o transporte é realizado por um robô móvel garantindo uma ausência de esforço físico e mobilidade de pessoas entre cozinha e enfermaria, enquanto o servo-assistido é mais económico e fácil de implementar nos serviços de saúde existentes.

A utilização de protótipos virtuais, permitiu analisar dimensões, formas e realizar testes dinâmicos e simulações realistas que ajudam a apresentar o conceito, sem que fosse necessário dispensar verbas para o seu fabrico e aquisição de materiais e componentes.



ENGENHARIA QUÍMICA

Anuário Científico 2007

ISEL

SERVICE QUALITY DIMENSIONS IN PORTUGUESE HOTELS: A PILOT INVESTIGATION WITH CRITICAL INCIDENT TECHNIQUE

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Service customers perceive quality in the moment of interaction with the service provider and particularly valuable is to define and understand customers' requirements. This paper explores the dimensions of service quality in hospitality and recognizes the dimensions which tend to be primarily a source of satisfaction and others that tend to be a source of dissatisfaction. To obtain the information it was conducted a pilot study applying the critical incident technique (CIT). The paper provides an overview of the critical incident technique, their strengths and weaknesses and its use in service research. Using CIT, data were gathered from two Portuguese hotel guests in Algarve, regarding satisfying or dissatisfying episodes with the service provided. The identification of the service quality dimensions is very important to develop measures to assess these quality dimensions allowing hotel managers to improve the delivery of customer perceived quality during the provided service and also to have greater control over the outcome.

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*Working Paper
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AN ALTERNATIVE TO THE MUSA METHOD FOR CUSTOMER SATISFACTION ANALYSIS

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This paper presents a critical analysis of MUSA method and introduces an alternative one. The aggregation method of the individual customer satisfaction criteria into an overall value function uses dummy variable regression techniques with additional constraints and employs the least squares approach for running the regression. The value of each level of the value function is calculated considering that each dummy variable coefficient represents the difference of value of that level to a reference level. The plot of the value functions and the relative weights provide a basis for a straightforward interpretation of the results. An illustrative example shows the differences observed between the models.

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Working Paper CEG-IST, 2007, 20, 1-27 (ISSN 1646-295).

Coriolus versicolor SUPPLEMENTATION IN CIN-1 (LSIL) HPV INFECTION: MODE OF ACTION

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Human papilloma viruses (HPV) are small, non-enveloped viruses containing a double-stranded DNA genome of around 8Kb. They are considered to be highly host-specific and infect epithelial cells. There are some 100 strains of HPV in all with different genotypes, one small group of which has been identified as being responsible for certain types of tumours in different epithelia. This group of HPV is the number one cause of cervical cancer (carcinoma). Other HPV strains cause genital warts and have led to HPV sometimes being called the wart virus or genital wart virus. However, the types of HPV that cause warts are not the types that cause cervical cancer.

There are 13 sub-types of HPV that are considered “high risk” for cervical cancer, including HPV 16, 18, 31 and 45. Of these, HPV 16 and HPV 18 are thought to be responsible for 70% of the cases of cervical cancer. High risk types can cause changes in the cells covering the cervix that make them more likely to become cancerous in time. If a patient has persistent or frequent infections with any of the ‘high risk’ types they are at risk of developing pre-cancerous cervical cells or cervical cancer.

Cervical cancer usually affects women between the ages of 35 and 55. Risk for cervical cancer seems to increase as a woman’s age at first sexual intercourse decreases and as the number of sexual partners increases. Failure to have a regular Pap test also increases risk. Eighty-five (85) percent of cervical cancers are squamous cell carcinomas, which develop in the scaly, flat, skin like cells covering the outside of the cervix. The remaining 15% of cervical cancers develop from gland cells (adenocarcinomas) or a combination of cell types (adenosquamous carcinomas).

Publicado em:
*Clinical Journal of
Mycology, 2007,
2 (Ed.1), 6-10.*

STRUCTURE OF AMIDASE FROM *Pseudomonas aeruginosa* SHOWING A TRAPPED ACYL TRANSFER REACTION INTERMEDIATE STATE

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Publicado em:
Journal of Biological Chemistry, 2007, 287(27), 598-605.

Microbial amidases belong to the thiol nitrilases family and have potential biotechnological applications in chemical and pharmaceutical industries as well as in bioremediation. The amidase from *Pseudomonas aeruginosa* is a 6 x 38-kDa enzyme that catalyzes the hydrolysis of a small range of short aliphatic amides. The hereby reported high resolution crystallographic structure shows that each amidase monomer is formed by a globular four-layer $\alpha\beta\beta\alpha$ sandwich domain with an additional 81-homologous C-terminal chain of another monomer, producing a strongly packed dimer. In the crystal, the biological active homohexameric amidase is built grouping three such dimers around a crystallographic 3-fold axis. The structure also elucidates the structural basis for the enzyme activity, with the nitrilases catalytic triad at the bottom of a 13-Å deep, funnel shaped pocket, accessible from the solvent through a narrow neck with 3-Å diameter. An acyl transfer intermediate, resulting from the purification protocol, was found bound to the amidase nucleophilic agent, Cys¹⁶⁶. These results suggest that some pocket defining residues should undergo conformational shifts to allow substrates and products to access and leave the catalytic pocket, for turnover to occur.

CRYSTALLIZATION DIFFRACTION DATA AND PRELIMINARY CRYSTALLOGRAPHIC ANALYSIS OF HEXAGONAL CRYSTALS OF *Pseudomonas aeruginosa* AMIDASE

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The aliphatic amidase (acylamide amidohydrolase; EC 3.5.1.4) from *Pseudomonas aeruginosa* is a hexameric enzyme composed of six identical subunits with a molecular weight of ~38kDa. Since microbial amidases are very important enzymes in industrial biocatalysis, the structural characterization of this enzyme will help in the design of novel catalytic activities of commercial interest. The present study reports the successful crystallization of the wild-type amidase from *P. aeruginosa*. Native crystals were obtained and a complete data set was collected at 1.4 Å resolution, although the crystals showed diffraction to 1.25 Å resolution. The crystals were found to belong to space group $P6_322$, with unitcell parameters $a = b = 102.60$, $c = 151.71$ Å, and contain one molecule in the asymmetric unit.

Publicado em:
Acta Crystallographica,
2007, F63, 214-216.

MONOCLONAL ANTIBODIES RECOGNIZE CONFORMATIONAL EPITOPES ON WILD-TYPE AND RECOMBINANT MUTANT AMIDASES FROM *Pseudomonas aeruginosa*

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Publicado em:

*Molecular
Biotechnology, 2007,
37, 136-145.*

Hybridoma technology was used to raise monoclonal antibodies (MAbs) against wild-type amidase from *Pseudomonas aeruginosa*. Hybridoma clones secreting polyol-responsive MAbs (PR-MAbs) were screened that bind antigen tightly but release under mild- and non-denaturing elution conditions, which can be used as ligands in immunoaffinity chromatography. Two of these hybridoma clones (C9E4 and B1E4) secreting MAbs against wild-type amidase were selected in order to check if they are PR-MAbs by using ELISA-elution assay. These hybridoma cell lines secreted MAbs of IgG class which were purified in a single step by Protein A-Sepharose CL-4B chromatography, which revealed two protein bands on SDS-PAGE. Specificity studies of MAb C9E4 revealed that it recognized a common epitope on wild-type and mutant T103I amidases as determined by direct ELISA, as well as by Western blotting under native conditions. This MAb exhibited a higher-affinity constant (K) for the mutant T103I amidase than for the wild-type enzyme. However, this MAb did not recognize either wild-type or mutant T103I enzymes under denaturing conditions suggesting that it binds to a conformation-sensitive epitope on amidase molecule. On the other hand, it also does not recognize either native or denatured forms of mutant C91A amidase suggesting that this substitution disrupted the conformational epitope present on amidase molecule. Furthermore, MAb C9E4 inhibited about 80% of wild-type amidase activity, whereas it activated about 80% of mutant amidase (T103I) activity. However, this MAb did not affect mutant C91A amidase activity which is in agreement with other results presented in this work. The data presented in this work suggest that this MAb acts as a powerful probe to detect conformational changes in native and denatured amidases as well as to differentiate wild-type and mutant (T103I and C91A) amidases.

PRODUCTION OF POLYGALACTURONASE FROM *Coriolus versicolor* GROWN ON TOMATO POMACE AND ITS CHROMATOGRAPHIC BEHAVIOUR ON IMMOBILIZED METAL CHELATES

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Tomato pomace and pectin were used as the sole carbon sources for the production of polygalacturonase from a strain of *Coriolus versicolor* in submerged culture. The culture of *C. versicolor* grown on tomato pomace exhibited a peak of polygalacturonase activity (1.427U/l) on the third day of culture with a specific activity of 14.5U/mg protein. The production of polygalacturonase by *C. versicolor* grown on pectin as a sole carbon source increased with the time of cultivation, reaching a maximum activity of 3.207U/l of fermentation broth with a specific activity of 248U/mg protein. The levels of different isoenzymes of polygalacturonase produced during the culture growth were analysed by native PAGE. Differential chromatographic behaviour of lignocellulosic enzymes produced by *C. versicolor* (i.e. polygalacturonase, xylanase and laccase) was studied on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion were studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The adsorption of these lignocellulosic enzymes onto immobilized metal chelates was pH-dependent since an increase in protein adsorption was observed as the pH was increased from 6.0 to 8.0. The adsorption of polygalacturonase as well as other enzymes to immobilized metal chelates was due to coordination of histidine residues which are available at the protein surface since the presence of imidazole in the equilibration buffer abolished the adsorption of the enzyme to immobilized metal chelates. A one-step purification of polygalacturonase from *C. versicolor* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II) and purified enzyme exhibited a specific activity of about 150U/mg protein, final recovery of enzyme activity of 100% and a purification factor of about 10. The use of short spacer arm and the presence of imidazole in equilibration buffer exhibited a higher selectivity for purification of polygalacturonase on this column with a high purification factor. The purified enzyme preparation was analysed by SDS-PAGE as well as by “*in situ*” detection of enzyme activity.

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Journal of Industrial & Microbiology & Biotechnology
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THE IMPORTANCE OF CONSIDERING BUILDING DOWNWASH WHEN ASSESSING THE NEED TO HEIGHTEN STACKS OF EXISTING SMALL AND MEDIUM SIZED INDUSTRIES

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Publicado em:
Clean Air, 2007, 8(1),
25-32.

This short communication intends to share the authors experience on the modelling of atmospheric pollutant dispersion and on the importance of building downwash considerations when assessing the need to increase the height of stacks of small and medium sized industrial facilities (SME's). In order to understand the reasons that make industrial companies, especially SME's, consider stack height, in section 2 the existing Portuguese legislation on air quality and the stack height rules are briefly commented. New legislation that ought to appear soon (new Portuguese Air Act) is also commented and compared critically with the existing one. Section 3 characterizes Portuguese industry in terms of ambient quality problems related to stack height. The adequacy of the stack height legislation to the particularities of the Portuguese case is discussed. In section 4 the authors experience in the specific study of stack height is presented. The methodology considered in these studies is discussed and compared to the application of existing and soon to appear legislation on stack height calculation. Finally, section 5 presents the conclusions and the need for an increased awareness on the pollutant dispersion problem is discussed.

NEW TECHNOLOGIES FOR EFFECTIVE FIRE FIGHTING

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Efficient fire extinction with water could be greatly improved by using superabsorbent polymers, added to the water used for fire fighting, or sprayed over surfaces of combustible materials in order to protect them from fire. Specially developed superabsorbent polymers such as acrylamide/2-acrylamide-2-methyl-propane-sulphonate (AA/AMPS) seem to be particularly efficient for this purpose. In terms of water absorption, the experimental tests performed, showed that the optimal composition of this polymer is 30:70 AMPS versus AA, using 0.5% of bis-acrylamide (BA) as crosslinking agent.

Publicado em:

International Journal of Environmental Studies, 2007, 64(2), 243-251.

DEVELOPING A LOCAL CARBON DIOXIDE EMISSIONS INVENTORY BASED ON ENERGY DEMAND AND WASTE PRODUCTION

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Publicado em:
*International Journal of
Environmental Studies,*
2007, 64(3), 347-355.

This paper reports the development of a carbon dioxide emissions matrix for the Oeiras municipality, one of the largest Portuguese municipalities, located in the metropolitan area of Lisbon. This matrix takes into account greenhouse gas emissions, caused by an increase of electricity demand in buildings as well as solid and liquid wastes treatment, from the domestic and service sectors. Using emission factors that were calculated from the relationship between the produced energy and amount of treated wastes, greenhouse gas emissions in the Oeiras municipality, were estimated for a time series of six years (1998 to 2003). The results obtained showed that the electricity sector accounts for about 75% of the municipal emissions in 2003. This study constitutes a tool to define sectors for appropriate action, including energy planning and also public information.

ASSESSING THE POSSIBILITY OF CORROSION OCCURRENCE IN METALLIC STACKS CAUSED BY HYDROCHLORIC ACID

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This article presents a simple method to estimate the possibility of corrosion in metallic stacks and surfaces due to hydrochloric acid deposition from stack gases, based on the HCl content in gases and also the flue gas temperature.

Publicado em:
*Chemical Engineering
Communications,*
2007, 194(6), 754-759.

DEVELOPMENT OF A LOCAL CARBON DIOXIDE EMISSIONS INVENTORY BASED ON ENERGY DEMAND AND WASTE PRODUCTION

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This paper describes the study that led to the development of a carbon dioxide emissions matrix for the Oeiras municipality, one of the largest Portuguese municipalities, located in the metropolitan area of Lisbon. This matrix takes into account the greenhouse gas (GHG) emissions due to an increase of electricity demand in buildings as well as solid and liquid wastes treatment from the domestic and services sectors. Using emission factors that were calculated from the relationship between the electricity produced and amount of treated wastes, the GHG emissions in the Oeiras municipality were estimated for a time series of 6 yr (1998-2003). The obtained results showed that the electricity sector accounts for approximately 75% of the municipal emissions in 2003. This study was developed to obtain tools and actions to be undertaken by local authorities such as energy planning and also public information.

Publicado em:

Journal of Air and Waste Management Association, 2007, 67, 1032-1037.

REFLECTIONS ON THE USE OF MC CABBÉ AND THIELE METHOD

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This paper reflects on the continuity of teaching the McCabe and Thiele method on chemical engineering courses for understanding the vapour-liquid equilibrium phenomena involved in distillation. Some exercises comparing the results obtained by this method as well as by other accurate analytical methods are presented and solved, as they are taught in ISEL courses. Because of its accuracy and easiness of use, and also because of the fact as this method allows an easy visualisation of the whole operation itself, the McCabe and Thiele method continues to be widespread used and students show a remarkable adherence to it.

Publicado em:
*Revista Ciências &
Tecnologia da
Universidade de
Pernambuco, 2007,
1, 1-7.*

MEASUREMENTS OF INDOOR AIR POLLUTANT LEVELS IN A UNIVERSITY OFFICE BUILDING

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Publicado em:
*Journal of Green
Building, 2007, 2(4),
123-129.*

This work consisted of a series of determinations performed in typical rooms of a building belonging to the Technical University of Lisbon, which is located in a central urban area of Lisbon. The main objective was to evaluate the Indoor Air Quality (IAQ) of the rooms so that further corrective measures could be taken if unsatisfactory IAQ levels were to be found. Correlations were derived, between indoor and outdoor pollutant concentrations, in order to assess the existence of contaminations coming from outside. Also, correlations were derived between total volatile organic compounds (VOC) concentrations and specific individual organic species measured in the same room. The methodology recorded in this paper is effective to assess compliance analysis of total VOCs, however, it seems somewhat limited to determine specific individual chemical species responsible for obtaining high total VOC concentrations.

ESTIMATIVA DA CORROSÃO EM CHAMINÉS METÁLICAS POR ÁCIDO CLORÍDRICO

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Este trabalho descreve um método simples de estimar a possibilidade da ocorrência de corrosão em chaminés metálicas devido à condensação de ácido clorídrico, baseado na determinação do teor de HCl e na temperatura dos gases.

Publicado em:

Ingenium, 2007, 97,
124-125.

EMIÇÃO DE MICROPOLUENTES ORGÂNICOS (DIOXINAS, DIBENZOFURANOS, PAHS E PCBS) NO FABRICO DE AÇO EM FORNO DE ARCO ELÉCTRICO

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Neste artigo descreve-se o estudo dos mecanismos de formação e destruição de compostos orgânicos de elevada toxicidade, tais como dioxinas, dibenzofuranos, PAHs e PCBs, no processo de fabrico de aço por arco eléctrico. Este estudo visa relacionar o nível das emissões destes compostos com variáveis operacionais que sejam consideradas como críticas, no sentido de possibilitar a redução dessas mesmas emissões através de um adequado controlo do processo.

Publicado em:

Ingenium, 2007, 97,
144-148.

AVALIAÇÃO EXPEDITA DA POSSIBILIDADE DE OCORRÊNCIA DE CORROSÃO EM CHAMINÉS METÁLICAS

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Os gases ácidos provocam frequentemente corrosão acentuada em chaminés metálicas. Neste trabalho apresenta-se um método de avaliação expedita da possibilidade de ocorrência desse tipo de corrosão provocada por efluentes gasosos contendo óxidos de enxofre e que se baseia na estimativa do ponto de orvalho dos gases como função das concentrações de trióxido de enxofre e vapor de água medidas na emissão.

Publicado em:
Ingenium, 2007, 97,
154-155.

MÉTODOS EXPEDITOS DE ESTIMATIVA DA CONCENTRAÇÃO DE POLUENTES GASOSOS NO INTERIOR DE EDIFÍCIOS

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Publicado em:
Engenharia Química,
2007, 6, 56-59.

Neste trabalho apresentam-se métodos, de fácil aplicação, que permitem determinar, de forma expedita, as concentrações no interior de edifícios de substâncias tóxicas devidas a emissões extemporâneas. Apresentam-se, igualmente, exemplos de aplicação que permitem responder ainda a problemas típicos que se colocam relativamente à ventilação de edifícios, como sejam a quantificação das taxas de renovação necessárias para fazer a exaustão de gases tóxicos acumulados no interior dos edifícios, ou como proceder para evitar a contaminação de gases vindos do exterior.

OPTIMIZAÇÃO DA REACÇÃO DE SÍNTESE DE HIDROXIAPÁTITE POR PRECIPITAÇÃO AQUOSA

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A hidroxiapatite (HAP) é um material biocerâmico amplamente utilizado em aplicações médicas e no revestimento de próteses metálicas ou preenchimento de cavidades nos tecidos duros do corpo resultantes de traumatismos ou de doenças. A HAP pode ser produzida por diferentes métodos, nomeadamente por processos hidrotérmicos, de precipitação ou de sol-gel, etc. A HAP no contexto deste estudo foi produzida por precipitação a partir de soluções de Ca(OH)_2 (0,5M) e de H_3PO_4 (0,3M) variando a temperatura reaccional, o pH, o caudal de adição de ácido, a velocidade de agitação e o grau de inertização. Os produtos resultantes foram secos e posteriormente sinterizados, e caracterizados por IV, difracção de raios X (DRX) e Microscopia Electrónica de Varrimento (SEM). A HAP apresenta uma pureza elevada, é estequiométrica e termicamente estável quando sintetizada a um pH entre 7 e 9, à temperatura reaccional de 60°C num meio adequadamente inertizado. As nano partículas de HAP sintetizadas são idênticas às biológicas permitindo a sua produção industrial para utilização na aplicação de implantes ósseos.

Publicado em:

Ciência e Tecnologia de Materiais, 2007, 19(3/4), 75-82.

SOBRE A CONTINUIDADE DO USO DO MÉTODO DE MC CABE AND THIELE

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Publicado em:
Engenharia Química,
2007, 7, 48-52.

Neste artigo tecem-se considerações sobre a continuidade do ensino do método de McCabe e Thiele nos cursos de engenharia química para compreender o fenómeno do equilíbrio líquido-vapor que regula a destilação. Apresentam-se problemas, leccionados nos cursos do ISEL, em que os resultados dados por este método são comparados com outros métodos analíticos. Devido á sua precisão e facilidade de uso, e ainda porque este método permite uma fácil visualização da operação unitária, este método continua a ser leccionado e os alunos mostram uma grande aptidão para a sua utilização.

MÉTODOS EXPEDITOS DE ESTIMATIVA DA CONCENTRAÇÃO DE POLUENTES GASOSOS NO INTERIOR DE EDIFÍCIOS

Gomes, J.F.

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Neste trabalho apresentam-se métodos, de fácil aplicação, que permitem determinar, de forma expedita, as concentrações no interior de edifícios de substâncias tóxicas devidas a emissões extemporâneas. Apresentam-se, igualmente, exemplos de aplicação que permitem responder ainda a problemas típicos que se colocam relativamente à ventilação de edifícios, como sejam a quantificação das taxas de renovação necessárias para fazer a exaustão de gases tóxicos acumulados no interior dos edifícios, ou como proceder para evitar a contaminação de gases vindos do exterior.

Publicado em:

Ingenium, 2007, 101,
68-70.

STUDY OF METAL–NH₃ INTERFACES (METAL = Cu, Ni, Ag) USING POTENTIOSTATIC CURVES

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Students determine kinetic and thermodynamic parameters of different metal-solution interfaces. These parameters are obtained from potentiostatic curves using the Tafel and the Arrhenius equations. The work involves the variation of type of metal, solution concentration, and temperature. The results allow the discussion of the polarizability, transfer coefficient, and activation energy of the processes, as well as the differences between them.

Publicado em:

*Journal of Chemical
Education, 2007, 84,
1017-1020.*

DETERMINATION OF SOLVATION AND SPECIFIC INTERACTION ENTHALPIES OF ADAMANTANE DERIVATIVES IN APROTIC SOLVENTS

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Solution and solvation enthalpies at infinite dilution of 1-bromoadamantane, 1-adamantanol, and 2-adamantanone are reported at 298.15K in a set of 14 aprotic solvents. The specific interaction enthalpies of the solid solutes are calculated using a methodology recently published by other authors. 1-Adamantanol's specific interaction enthalpies show a good correlation with the Kamlet-Taft β scale.

Publicado em:

*Journal of Chemical
Thermodynamics,*
2007, 39, 1201-1205.

ENZYMATIC DECOLOURISATION AND DETOXIFICATION OF THE AZO DYE SUDAN ORANGE G WITH BACTERIAL CotA-LACCASE

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Publicado em:
*Journal of
Biotechnology*, 131S
(2007), pp. S107-S108.

Enzymatic bioremediation has become an attractive alternative to support the bio-treatment techniques currently available as enzymes provide simpler systems than a whole organism and could be improved by the use of modern engineering techniques by using rational (site-directed mutagenesis), semirational (*i.e.* combinatorial saturation mutagenesis) and directed evolution approaches. Laccases constitute a large subfamily of multicopper oxidases and have a great potential in various biotechnological processes mainly due to their high relative non-specific oxidation capacity, the lack of a requirement for cofactors, and the use of readily available oxygen as an electron acceptor.

Fungal laccases have been confirmed for its ability to decolourise a wide number of azo and anthraquinone dyes. These dyes account for more than 50% of all dyes in the textile, food, pharmaceutical, leather, cosmetics and paper industries and therefore, azo dyes are the most common synthetic colorants released into the environment. Colour removal from wastewaters with traditional physical-chemical processes, such as coagulation, adsorption and oxidation with ozone are unable to degrade all dyes currently used and these compounds are generally resistant to degradation by biological treatment methods. Furthermore, some of the aromatic amines generated these biological processes are toxic and carcinogenic.

In this study, enzymatic degradation of the azo dye Sudan Orange and of the anthraquinone dye Acid Blue 62 was examined. The CotA-laccase is a bacterial laccase from *Bacillus subtilis* that has been extensively studied at the molecular level. The main objectives of such studies are to dissect the catalytic mechanisms and to design laccases that better match biotechnological applications, using protein engineering techniques. Only little information is available about the reactivity of azo and anthraquinonic dyes and the nature of their degradation products. Moreover, their products may be more toxic than the original compound. The kinetics of azo and anthraquinonic dyes oxidation was studied and the main products were separated by HPLC and identified by NMR and MS. The possible mechanisms involved in the degradation are discussed. Finally, we have examined the toxicity of the degradation products.

INFLUENCE OF STEAM HEATING ON THE PROPERTIES OF PINE (*PINUS PINASTER*) AND EUCALYPT (*EUCALYPTUS GLOBULUS*) WOOD

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Heat treatment of *Pinus pinaster* and *Eucalyptus globulus* woods, two important species in Portugal, was performed in the absence of air by steaming, inside an autoclave, for 2–12h at 190–210°C. Mass losses increased with treatment time and temperature reaching 7.3% for pine and 14.5% for eucalypt wood. The wood behaviour with moisture was improved. The equilibrium moisture content decreased by 46% for pine and 61% for eucalypt, the dimensional stability increased (maximum anti-shrinking efficiency in the radial direction of 57 and 90% for pine and eucalypt, respectively) and the surface wettability was lowered. In relation to mechanical properties, the modulus of elasticity was little affected (maximum decrease of 5% for pine and 15% for eucalypt) but the bending strength was reduced (by 40% at 8% mass loss for pine and 50% at 9% mass loss for eucalypt wood). The variation of properties was related to treatment intensity and mass loss but significant improvements could already be obtained for a 3–4% mass loss without impairing the mechanical resistance. The response of eucalypt was higher than that of pinewood. Heat treatment of eucalypt wood shows an interesting potential to improve the wood quality for solid timber products.

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HEAT-INDUCED COLOUR CHANGES OF PINE (*PINUS PINASTER*) AND EUCALYPT (*EUCALYPTUS GLOBULUS*) WOOD

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Heat treatment of *Pinus pinaster* and *Eucalyptus globulus* wood was carried out by hot air in an oven for 2–24 h at 170–200°C and by steam in an autoclave for 2–12 h at 190–210°C. The colour parameters L^* , a^* and b^* were determined by the CIELAB method on radial, tangential and transverse sections of untreated and treated wood, and their variation with regard to the treatment (DL^* , Da^* and Db^*) were calculated in percent. For untreated eucalypt wood, lightness (L^*) varied between 54.1 and 63.8% with a^* between 7.4 and 8.5, and b^* between 15.7 and 19.9. For untreated pinewood, L^* varied between 67.3 and 76.1%, a^* between 6.9 and 7.6 and b^* between 16.3 and 24.1. Oven heat-treated wood became darker (DL^* about 50% for 4% mass loss), and this was more for eucalypt wood under the same treatment conditions. In general, the contribution of red (a^*) and yellow (b^*) colour decreased with heat treatment. The transverse section of the two species darkened less for both the treatments with small differences between radial and tangential sections. Lightness decrease was related to chemical changes; with good correlations with glucose ($R_2 = 0.96$), hemicelluloses ($R_2 = 0.92$) and lignin ($R_2 = 0.86$). As regards colour, the heat treatments showed an interesting potential to improve the wood quality for solid timber products from pine and eucalypt.

IMPROVEMENT OF TOLUENE CATALYTIC COMBUSTION BY ADDITION OF CESIUM IN COPPER EXCHANGED ZEOLITES

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HYand HMFI zeolites exchanged with copper and cesium have been studied for the catalytic combustion of toluene (800ppm) with air. The catalysts activity has been analyzed by comparison of light-off curves and in both Cu zeolites, the addition of Cs leads to a decrease of the light-off temperature by 50 8C. Temperature-programmed reduction (H₂-TPR) and EPR studies have evidenced clear differences in the characteristics of the copper species both in the presence and absence of Cs co-cations. These differences account for the nature of the active centers in the Cu zeolites for the toluene oxidation. The position and geometry of the copper ions in the zeolite matrix are of great significance for the redox behavior and activity for toluene oxidation. In both MFI and FAU structures, the bulky Cs co-cations are located in the more accessible main zeolite pores, forcing the copper ions to occupy the most stable, but less accessible positions within each structure. In the case of the MFI zeolite, the EPR study revealed that the Cs exchange resulted in an increased abundance in the number of square pyramidal Cu²⁺ ions relative to the other Cu environments. Cs cocations also lead to an increase in the reducibility of the copper ions mainly due the reduction of protons in Cu, Cs-containing samples.

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MANUFACTURE OF CORDIERITE FOAMS BY DIRECT FOAMING

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Open cell cordierite foams were prepared by a direct foaming two-component polyurethane (PUR)/ceramic system. Through optimization of several experimental parameters, such as contents of catalyst, and ceramic cordierite precursor, as well plasticizer presence, foams with porosities 85–95% and densities ranging from 130–410kg ·m were obtained. These foams characteristics make them attractive to be used as catalyst supports. The new two-component PUR/ceramic system developed allows the high solid's loading (higher than 40wt.%). Finer ceramic particles in this system provide better particles' package and cohesion upon sintering, favouring the cordierite foam stability.

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*Polimery, 2007, 52
(5), 31-36.*

ACIDITY CHARACTERIZATION OF PILLARED CLAYS THROUGH MICROCALORIMETRIC MEASUREMENTS AND CATALYTIC ETHYLBENZENE TEST REACTION

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The catalytic disproportionation of ethylbenzene, a test reaction that was proposed in the literature for the characterization of the acidity of zeolitic materials, was used for the evaluation of the surface acidity of pillared clays. The catalytic behaviour was correlated with the results of the surface acidity characterization made by adsorption microcalorimetry of aromatic molecules and pyridine. The aromatic probe molecules used were a reactant and a product of the catalytic reaction: ethylbenzene and meta-diethylbenzene, respectively. In this way, only the accessible and strongest acid sites are titrated. The heats of adsorption of these molecules indicate that a zirconium oxide pillared clay has stronger acidity than an aluminium oxide pillared clay whereas pyridine results are equal for both samples. The difference in surface acidity, assessed by ethylbenzene and meta-diethylbenzene, correlates well with the initial catalytic activity of the materials which is higher in the zirconium sample than in the aluminium sample. These observations show that both methodologies, that is, the catalytic test reaction and the adsorption microcalorimetry of selected aromatic molecules, are useful for the surface acidity characterization of pillared clays.

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DENSITY MEASUREMENTS OF FLUIDS AND THEIR MIXTURES AT HIGH PRESSURE

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and Technology, 2007,
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The principles of the isochoric method are described, as well as the different variants of this method that can be considered according to the technique used to determine the amount of fluid inside the high pressure cell. An automated isochoric apparatus to measure the density of binary mixtures is presented. Accurate isochoric measurements of density of pure fluids, involving molecules like methanol, and mixtures, such as nitrogen plus methane and a multicomponent system with a composition representative of the U.S.A. commercial Gulf Coast natural gas, are analyzed. Moreover, the effect of the thermal degradation of fluids at high temperatures on the accuracy of the density measurements is also discussed.

SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF VOLATILES FROM *SATUREJA FRUTICOSA* BÉGUINOT

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Dried flowers and leaves of *Satureja fruticosa* Béguinot were submitted to supercritical CO₂ extraction (SFE) followed by a two stage fractional separation. The extraction was carried out at 40°C in a flow apparatus, provided with a 1L extraction vessel and two separators of 0.27L each. Conditions of extraction, such as pressure, particle size of plant material and CO₂ flow rate, were studied in order to assess their influence on the yield and composition of the volatiles. The best conditions of extraction were 9obar pressure at 1.32Kg/h of CO₂ flow rate and a plant material particle size of 0.5mm. The SFE volatiles obtained and the essential oil isolated by hydrodistillation (HD) were analysed and compared by GC and GC-MS. The oxygen-containing monoterpenes, pulegone (33-36% for SFE and 40-41% for HD), isomenthone (14-18% for SFE and 21% for HD), piperitenone (11-12% for SFE and 9-11% for HD) and piperitenone oxide (11-13% for SFE and 7-9% for HD) were the dominant components in all samples.

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*Flavour and Fragrance
Journal*, 2007, 22,
438-442.

PYRAZOLE AND TRISPYRAZOLYLMETHANE RHENIUM COMPLEXES AS CATALYSTS FOR ETHANE AND CYCLOHEXANE OXIDATIONS

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 2007, 317, 43-52.

The pyrazole complexes $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})(\text{PPh}_3)_2]$ **2** (Hpz = pyrazole), $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})_2(\text{PPh}_3)]$ **3** and $[\text{ReClF}\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})_2(\text{PPh}_3)]$ **4**, and the tris(pyrazoly)methane compounds $[\text{ReCl}_2(\text{HCpz}_3)(\text{PPh}_3)]$ **5** (pz = pyrazolyl), $[\text{ReCl}_3\{\text{HC}(\text{pz})_3\}]$ **7**, $[\text{ReOCl}_2\{\text{SO}_3\text{C}(\text{pz})_3\}(\text{PPh}_3)]$ **8** and $[\text{ReO}_3\{\text{SO}_3\text{C}(\text{pz})_3\}]$ **9**, and their precursors $[\text{ReCl}_2\{\eta^2\text{-N},\text{O}-\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{PPh}_3)_2]$ **1** and $[\text{ReOCl}_3(\text{PPh}_3)_2]$ **6**, act as selective catalysts (or catalyst precursors), in a single-pot process, for the oxidation of ethane, in the presence of potassium peroxodisulfate $\text{K}_2\text{S}_2\text{O}_8$, in trifluoroacetic acid (TFA), to give acetic acid, in a remarkable yield (up to ca. 40%) and under mild conditions (in some cases carboxylation can also occur to give propionic acid, but in a much lower yield). The catalytic peroxidative oxidation of ethane to acetaldehyde and of cyclohexane to cyclohexanone and cyclohexanol by an aqueous solution of H_2O_2 at room temperature is also achieved by using most of those catalyst precursors. The effects of a variety of factors were studied towards the optimization of the processes which are shown to proceed via both C-centered and O-centered radical mechanisms.

ARENERUTHENIUM(II) 4-ACYL-5-PYRAZOLONATE DERIVATIVES: COORDINATION CHEMISTRY AND REACTIVITY

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Skelton, B.W.²; White, A.H.²; Wanke, R.²;
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Areneruthenium(II) molecular complexes of formula [Ru(arene)(Q)Cl] containing 4-acyl-5-pyrazolonate ligands Q (HQ in general; in detail HQ^{nPe} is 1-phenyl-3-methyl-4-tert-butylacetyl-5-pyrazolone, HQ^{naph} is 1-phenyl-3-methyl-4-(2-naphthoyl)-5-pyrazolone, HQ^{CF3} is 1-phenyl-3-methyl-4-trifluoroacetyl-5-pyrazolone, HQ^{py,CF3} is 1-(2-pyridyl)-3-methyl-4-trifluoroacetyl-5-pyrazolone, HQ^{pent} is 1-phenyl-3-methyl-4-(4-pentenoyl)-5-pyrazolone and HQ^{Me,nPe} is 1,3-dimethyl-4-tert-butylacetyl-5-pyrazolone; arene = cymene or benzene) have been synthesized by the interaction of HQ and [Ru(arene)Cl(μ-Cl)]₂ dimers in methanol in the presence of sodium methoxide.) The dinuclear compound [{Ru(cymene)Cl}₂Q₄Q] (H₂Q₄Q = bis(4-(1-phenyl-3-methyl-5-pyrazolone) dioxohexane) has been prepared similarly by interaction of [Ru(cymene)Cl(μ-Cl)]₂ with H₂Q₄Q. [Ru(cymene)(Q)Cl] (Q = Q^{nPe} and Q^{py,CF3}) react with sodium azide in acetone affording [Ru(arene)(Q)N₃] derivatives, where Cl has been replaced by N₃⁻. The reactivity of the [Ru(cymene)(Q^{nPe})Cl] has also been explored toward monodentate donor ligands L (L = triphenylphosphine, 1-methylimidazole or 1-methyl-2-mercaptoimidazole) and exo-bidentate ditopic donor ligands L-L (L-L = 4,4'-bipyridine or bis(diphenylphosphino)propane) in the presence of silver salts AgX (X = SO₃CF₃ or ClO₄), new ionic mononuclear complexes of formula [Ru(cymene)(Q^{nPe})L]X and ionic dinuclear complexes of formula [{Ru(cymene)(Q^{nPe})₂L-L]X₂ being obtained. The solid-state structures of a number of complexes were confirmed by X-ray crystallographic studies. Their redox properties have been investigated by cyclic voltammetry and controlled potential electrolysis, which, on the basis of the measured Ru^{III/II} reversible oxidation potential, have allowed to order the bidentate acylpyrazolonate ligands according to their electron-donor character and are indicative of a small dependence of the HOMO energy upon change of the monodentate ligand. This is accounted for by DFT calculations which show a relevant contribution of acylpyrazolonate ligand orbitals to the HOMOs, while that from the monodentate ligand is minor.

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(20), 8245–8257.

BIS[HYDROTRIS (1-PYRAZOLYL)METHANE- $\text{K}^3\text{N},\text{N}',\text{N}''$] COPPER(II) CHLORIDE

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The reaction between copper(II) chloride dihydrate and excess of tris(1-pyrazolyl)methane results in formation of the title compound. The obtained complex crystallizes in monoclinic crystal system and has P21/c space group.

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m1979.

OPTIMIZATION OF "SERPA" CHEESE WHEY NANOFILTRATION FOR EFFLUENT MINIMIZATION AND BY-PRODUCTS RECOVERY

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Second cheese whey (SCW) is a by-product of cheese and curd cheese production that is usually not recovered and therefore substantially contributes to the negative environmental impact of the cheese manufacture plants. Membrane technology, namely nanofiltration (NF), is used in this work for the recovery of SCW organic nutrients, resulting from "Serpa" cheese and curd production.

The SCW is processed by NF to recover a rich lactose fraction in the concentrate and a process water with a high salt content in the permeate.

The permeation experiments were carried out in a plate & frame NF unit, where two NF membranes (NFT50 and HR-95-PP) were characterized and tested. The NF permeation experiments were performed accordingly with two different operation modes: total recirculation and concentration. In order to select the best membrane and operating pressure for the SCW fractionation, total recirculation experiments were carried out. The NF modeling was also performed, in terms of permeate fluxes and rejection coefficients using the resistances-in-series model and the solution-diffusion model, respectively. After the membrane selection, the concentration experiments showed that the selected membrane (NFT50) at 3.0MPa allows a water recovery of approximately 80%, concentrating the SCW nutrients approximately 5 times. Therefore, the NF operation can successfully reduce the wastewater organic load and simultaneously contributes to the valorization of the cheese and curd cheese manufacture by-products.

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THE ROLE OF EMERGENT TECHNOLOGIES TOWARDS AN INTEGRATED SUSTAINABLE ENVIRONMENT

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Most of the industrial production processes were developed in the 50's at the time of cheap and abundant raw materials, energy and water resources. The intensive use of water of good quality and the search for new processes/products aiming maximal profits led to scarcity and degradation of natural resources.

Reducing material waste is one of the greatest challenges facing industry today. Because water is one of the industry's major waste products, the ability to reduce waste water would be a giant step in the direction of overall waste reduction.

Water conservation and water use were considered justifiable only if they represented economic savings either in material recovering or in the avoidance of treatment costs. However, today's industrial facilities are constantly striving to operate more efficiently, and the most successful plans are relentless in their search for the following:

- | Higher product yields
- | Beneficial use of by-products
- | Improved energy efficiency
- | Safer and more reliable operations
- | Improved public image
- | Reduced environmental impacts

This paper provides a systematic approach with for outstanding examples from diverse industries: Corrugated board production industry; Dairy industry; Coke industry; Cork production industry.

The authors have combined the use of proven and accepted technologies and practices with some new emergent technologies developing a new systematic approach for minimizing net water usage at industrial facilities, presented it in a straight forward manner.

SURFACE PHOTOCHEMISTRY: BENZOPHENONE AS A PROBE FOR THE STUDY OF MODIFIED CELLULOSE FIBRES

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This work reports the use of benzophenone, a very well characterized probe, to study new hosts (*i.e.*, modified celluloses grafted with alkyl chains bearing 12 carbon atoms) by surface esterification. Laser-induced room temperature luminescence of air-equilibrated or argon-purged solid powdered samples of benzophenone adsorbed onto the two modified celluloses, which will be named C12-1500 and C12-1700, revealed the existence of a vibrationally structured phosphorescence emission of benzophenone in the case where ethanol was used for sample preparation, while a nonstructured emission of benzophenone exists when water was used instead of ethanol. The decay times of the benzophenone emission vary greatly with the solvent used for sample preparation and do not change with the alkylation degree in the range of 1500–1700 micromoles of alkyl chains per gram of cellulose. When water was used as a solvent for sample preparation, the shortest lifetime for the benzophenone emission was observed; this result is similar to the case of benzophenone adsorbed onto the “normal” microcrystalline cellulose surface, with this latter case previously reported by Vieira Ferreira *et al.* in 1995. This is due to the more efficient hydrogen abstraction reaction from the glycoside rings of cellulose when compared with hydrogen abstraction from the alkyl chains of the modified celluloses.

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*Research Letters in
Physical Chemistry,*
2007, 1-5.

COMPROMISE BETWEEN CONJUGATION LENGTH AND CHARGE-TRANSFER IN NONLINEAR OPTICAL η^5 -MONOCYCLOPENTADIENYLIRON(II) COMPLEXES WITH SUBSTITUTED OLIGO-THIOPHENE NITRILE LIGANDS: SYNTHESIS, ELECTROCHEMICAL STUDIES AND FIRST HYPERPOLARIZABILITIES

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A systematic series of η^5 -monocyclopentadienyliron(II) complexes with substituted oligo-thiophene nitrile ligands of general formula $[\text{FeCp}(\text{P}_\text{P})(\text{NC}\{\text{SC}_4\text{H}_2\}_n\text{NO}_2)]\text{PF}_6$ ($\text{P}_\text{P}=\text{dppe}$, (+)-diop; $n=1-3$) has been synthesized and characterized. The electrochemical behavior of the new compounds was explored by cyclic voltammetry. Quadratic hyperpolarizabilities (β) of the complexes with dppe coligands have been determined by hyper-Rayleigh scattering (HRS) measurements at two fundamental wavelengths of 1.064 and 1.550 μm , to uncover the two-photon resonance effect and to estimate static β values. The obtained overall results are found to be better than for the related η^5 -monocyclopentadienyliron(II) complexes with *p*-benzonitrile derivatives. Although an increase of the resonant β at 1.064 μm with increasing number of thiophene units in the conjugated ligand was found (up to 910×10^{-30} esu), the static values β_0 remain practically unchanged, as shown by the 1.550 μm measurements. Combined with the electrochemical and spectroscopic data (IR, NMR), and solvatochromism studies, this remarkable evolution of β shows that the increase of conjugation length is balanced by a decrease in charge-transfer efficiency.

ANÁLISE COMPARATIVA DO DESEMPENHO DE ARGILAS COM PILARES E ZEÓLITOS NA METILAÇÃO DO TOLUENO

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Com este trabalho pretende-se efectuar uma análise comparativa sob o ponto de vista estrutural, textural e desempenho catalítico de duas estruturas zeolíticas (HY e HZSM-5) uma argila natural proveniente de Porto Santo (PTS) e duas amostras obtidas por intercalação desta última com óxidos de Al e Zr.

As amostras foram caracterizadas estruturalmente por difracção de raios X de pós e texturalmente por adsorção de azoto a baixa temperatura. Na avaliação do desempenho catalítico dos sólidos foi realizada a reacção modelo de alquilação do tolueno pelo metanol. Nas PILCs a natureza dos pilares reflecte-se fundamentalmente nos valores do espaçamento basal, d_{001} . Todos os sólidos revelaram ser activos para a metilação do tolueno, mostrando que, mesmo só a acidez de Brönsted proveniente das camadas das argilas é suficiente para promover a alquilação. Como produtos maioritários desta reacção foram obtidos os isómeros xilenos (XY). Foram também detectados trimetilbenzenos (TMB) e etiltoluenos (EtT), dependendo os rendimentos dos respectivos isómeros da estrutura porosa e dimensionalidade do catalisador, ou seja com a correlação esperada, e concordante, com as respectivas texturas. Com excepção do HZSM-5 e da PTS constata-se o aparecimento de benzeno (B) nos produtos de reacção, indicando que a densidade de centros ácidos do HY e das argilas com pilares é suficiente para promover a dismutação do tolueno.

Publicado em:

Livros de Resumos do 8º Encontro Nacional de Catálise e Materiais Porosos da Sociedade Portuguesa de Química, Lamego, 21 a 23 de Setembro de 2007.

HIDROISOMERIZAÇÃO DE N-HEXANO SOBRE MISTURAS DE ZEÓLITOS OM Pt SUPORTADA EM MATERIAIS MESOPOROSOS

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Estudou-se o comportamento de catalisadores compósitos constituídos por zeólitos ácidos (MOR e BEA) e por Pt suportada em materiais mesoporosos (Al/SBA₁₅ e uma argila porosa heteroestruturada-PCH) na reacção de hidroisomerização de n-hexano. O desempenho catalítico destes materiais compósitos foi comparado com o dos mesmos materiais nos quais a Pt foi dispersa directamente, quer nos zeólitos ácidos, quer nos materiais mesoporosos.

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Portuguesa de
Química, Lamego,
21 a 23 de Setembro
de 2007.*

APPLICATION OF LSERS TO THE SOLUTION ENTHALPIES OF ADAMANTANE DERIVATIVES IN PROTIC AND APROTIC SOLVENTS AT 298.15K

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Recent studies have shown that adamantyl compounds and their derivatives evidence promising antibacterial and antiviral activity. This fact per se justifies a growing interest in the physicochemical characterization of these compounds, particularly the knowledge of their behaviour in solution. One of the most used techniques to study molecular interactions in solution is solution calorimetry. In a series of previous papers, we have reported solution enthalpies of 1-bromoadamantane in water-aprotic mixtures and in hydroxylic solvents. Also, the solution enthalpies at infinite dilution, sH^∞ , at 298.15K for three adamantane derivatives, namely 1-bromoadamantane (1-AdBr), 1-adamantanol (1-AdOH) and 2-adamantanone (2-AdO), in a set of aprotic solvents have been presented elsewhere. In this work, we integrate all the previously reported results and include a set of new solution enthalpies for the three referred adamantane derivatives in hydroxylic solvents. The thermochemical data are analyzed in terms of linear solvation energy relationships of the type $sH^\infty = f$ (solvent descriptors). This scrutiny showed that the consideration of a “true” cavity contribution is crucial for the rationalization of the differences observed for the three solutes.

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1 a 6 de Julho de
2007.*

REACTIVITY STUDIES OF TERTIARY ALKYL HALIDES IN METHANOL/ACETONITRILE AND METHANOL/1-PROPANOL: CORRELATION WITH MIXTURES' PROPERTIES

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2007.*

Due to the increased applications of mixed solvents in various fields, structural and dynamic studies using these solvents have gone through significant developments in the last few years. Solvent mixtures often exhibit complex behaviours deriving from multiple interactions in solution. As such, they represent an important tool to study solution phenomena since they are potentially more informative as the variability of most of their properties can be significantly increased through an adequate choice of components and compositions. Kinetic studies can be used as probes to address substrate-solvent-solvent interactions. Data for the heterolysis of 2-bromo-2-methylpropane in protic and aprotic solvent mixtures have been presented by us elsewhere. In this work, new rate constants, k , for the heterolysis of three other substrates, namely 2-iodo-2-methylpropane, 3-bromo-3-ethylpentane and 3-iodo-3-ethylpentane were determined at 25.00°C, using at least 10 mole fractions of the binary mixtures methanol/acetonitrile and methanol/1-propanol. A methodology involving correlation analysis among rate constants and suitable solvent descriptors allowed the identification and quantification of the major substrate-solvent-solvent interactions present in these reaction processes. Differences in the kinetic behaviour of the four substrates were also analysed.

SIMULTANEOUS TG-DSC ANALYSIS OF CONJUGATED CALIX[4]ARENE-BASED POLYMERS

Barata, P.D.; Costa, A.I.; Prata, J.V.

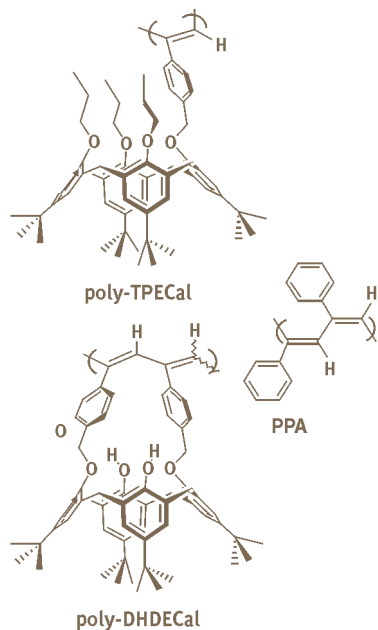
Dept. de Engenharia Química, ISEL, Lisboa, Portugal
C. de Inv. de Engenharia Química e Biotecnologia, ISEL, Lisboa, Portugal

The thermal induced reactions of highly stereoregular *cis*-transoidal poly(phenylacetylene) (PPA) have been studied in detail. A conformational change (*s-trans* to *s-cis*) followed by an electrocyclic ring-closing reaction of phenyl-substituted hexatriene sequences of the polymer chain have been proposed for *cis*-transoidal PPA.

Depending on the different bond breaking modes of the substituted cyclohexadiene units meanwhile formed, aromatic structures (e.g. 1,3,5-triphenylbenzene) are either extruded from the polymer with the simultaneous scission of the polymer chain, or incorporated on it (terphenylene units), with the concomitant release of benzene.

In this work, we report our preliminary results regarding the thermal behavior of novel conjugated polymers **poly-TPECal** and **poly-DHDECal**, having either a pendant or an incorporated calix[4]arene receptor along the main polyene chain, respectively, both synthesized in a living fashion using a Rh-based ternary catalytic system. The DSC traces of

each calix[4]arene-derived polymers show a clear exothermic event in the 308-334°C temperature range. On a second heating scan, the former exothermic phenomenon is absent, showing the irreversibility of the transition. It was also found that the aforementioned events occur with practically no weight loss of the polymer (TG curves corresponding to **poly-TPECal** and **poly-DHDECal**). In the case of **poly-DHDECal**, after it has been heated-up to 350°C, only a



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small fraction (*ca.* 2.5%) remains soluble in THF. Its GPC analysis showed however that it was mainly constituted by oligomeric materials. The FT-IR spectra of the thermal treated polymers resemble one another. A tentative interpretation of the results will be made.

THERMAL POLYMERIZATION OF SYN-DISTAL-DIPHENYLETHYNYL-CALIX[4]ARENE COMPOUNDS: A FT-IR AND DSC SCRUTINY

Costa, A.I.; Barata, P.D.; Prata, J.V.

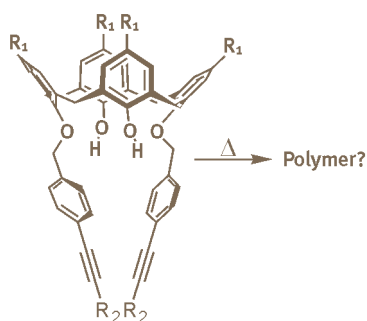
Dept. de Engenharia Química, ISEL, Lisboa, Portugal
C. de Inv. de Engenharia Química e Biotecnologia, ISEL, Lisboa, Portugal

The polymerization of calix[4]arenes **1** and **2** mediated by a Rh(I) catalyst was very recently reported. Under the conditions used, conjugated polymers were smoothly produced in good yields. Their high solubility in common nonprotic organic solvents, along with the unimodal GPC profiles (number-average molecular weights up to 1.1×10^5

gmol^{-1} ; $M_{n(\text{GPC})}$) led to the mechanistic proposal of a cyclopolymerization route, involving an alternating intra-intermolecular propagation chain mechanism.

As part of an ongoing project aiming to study the polymerizabilities of calix[4]arenes **1-4**, their thermal induced bulk polymerization was examined. Thus, for example, when calix[4]arene **2** was heated to 350°C under nitrogen ($10^\circ\text{C}/\text{min}$), at least three discrete events appear in

the DSC thermogram. An endothermic peak appear at 159.5°C (onset at 147.2°C) which should correspond to the melting point of **2**. Some decomposition of the material should also occur concomitantly during this transition, as could be noted in the TG curve (around 10% weight loss). Immediately following, a sharp exothermic event takes place, peaking at 193°C (end of transition *ca.* 210°C). This event should be related to the thermal polymerization of the melted compound. Indeed, the infra-red spectrum of a sample produced under similar conditions showed that the ethynylic stretching frequencies ($-\text{C}\equiv\text{C}-\text{H}$ and $-\text{C}\equiv\text{C}-$) were both absent. In addition, no mass loss was discernible in the TG during the transition. Further heating of the sample lead to another exothermic transition at 313°C , which was interpreted as a result of additional reactions between some of the ene components of the formed polymer (pericyclic or radical on its origin). A similar exothermic transition appears in the DSC trace of



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2007.*

the polymers obtained through the Rh(I) ca-talyzed polymerization of **2**. The materials thus obtained were analyzed by FT-IR and their soluble fractions were checked by GPC. The thermal induced polymerization of compounds **1, 3-4**, was carried out in an identical fashion and the results will also be presented.

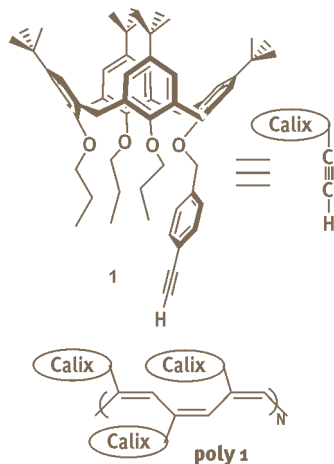
LIVING POLYMERIZATION OF TRI-*O*-PROPYL-(4-ETHYNYL)BENZYLOXY-*p*-*t*-BUTYLCALIX[4]ARENE BY A Rh-BASED TERNARY CATALYTIC SYSTEM: SYNTHESIS OF A NOVEL CONJUGATED CALIXARENE POLYMER WITH CONTROLLED MOLECULAR WEIGHT AND MWD

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The living polymerization of monosubstituted phenylacetylenes (PAs) using Rh(I) catalysts has been accomplished with three different catalytic systems. Noyori *et al.* first reported that Rh(C≡CPh)(nbd) (PPh₃)₂/4-DMAP and [Rh(nda)(OMe)]₂/PPh₃/4-DMAP systems promote the living polymerization of PA, with initiation efficiencies (I_{eff}) of 37% and 72%, respectively. New ternary catalyst systems of the type [Rh(diene ligand)Cl]/(Ar)₂-C=C-(Ar)H/P(4-R-C₆H₄)₃ (R=H, F, Cl), achieving quantitative I_{eff} , were later developed by Masuda *et al.*

As part of our ongoing research aiming to produce well-defined calixarene-based conjugated polymers as new materials for use in sensing chemistry, combining the molecular recognition capabilities of the calixarene scaffolds with the unique properties provided by the conjugated main chain polyene, the polymerization of tri-*O*-propyl-(4-ethynyl)benzyloxy-*p*-*t*-butylcalix[4]arene (**1**) was examined. Previous work with this monomer, prepared through a Sonogashira-Hagihara cross-coupling procedure previously developed by us, had shown that the polymerization sluggishly proceeds in toluene or



THF when [Rh(nbd)Cl]₂ was used, with or without added cocatalysts (PPh₃ and/or NHET₂). For instance, at a [Rh]:[monomer] molar ratio of 100:1 in toluene, the yield of the polymer was only 9%, in addition to *ca.* 30% of oligomeric products and 61% of starting **1**, after 5h at 30°C. A remarkable effect was witness when **1** was polymerized by a ternary catalytic system prepared *in situ* from [Rh(nbd)Cl]₂, 1,1-diphenyl-2-phenylvinyl lithium and PPh₃ in toluene, not only in the

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polymerization yield, which was quantitative (GPC analysis), but also in its selectivity, since no oligomeric materials were formed. Using different catalyst-to-monomer molar ratios (200:1; 100:1; 50:1 and 25:1), a linear relationship could be obtained between the number-average molecular weight ($M_{n(\text{GPC})}$) of **poly 1** and the [Rh]:[**1**] feed ratio, showing that the polymerization of **1** has proceeded in a living fashion. High I_{eff} and narrow polydispersities were achieved with this ternary system.

EFFICIENCY OF Rh-BASED TERNARY CATALYTIC SYSTEMS IN THE POLYMERIZATION OF TRI-*O*-PROPYL-(4-ETHYNYL)BENZYLOXY-*p*-*t*-BUTYLCALIX[4]ARENE

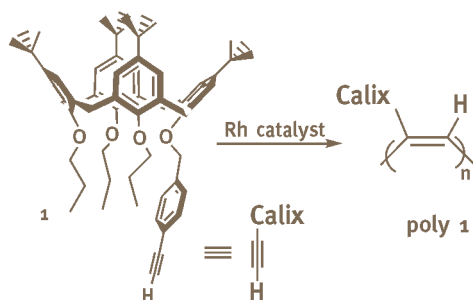
Costa, A.I.; Prata, J.V.

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The synthesis of well-defined calixarene-based polymers as new materials for sensing devices, together with its characterization and properties evaluation are current research topics in our laboratory. The synthesis of conjugated calix[4]arene polymers comprising 1,3-(4-ethynyl)benzyloxy-*p*-*t*-butylcalix[4]arene units along the main-chain was recently described. The aforementioned monomer underwent a smooth polymerization when $[\text{Rh}(\text{nbd})\text{Cl}]_2$ was used as catalyst and PPh_3 as an additive. Under appropriate conditions, high conversions

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were obtained and the resulting polymers, isolated in high yields, showed monomodal MWD and less than 5% of dimeric and oligomeric materials. On the contrary, when the polymerization of tri-*O*-propyl-(4-ethynyl)benzyloxy-*p*-*t*-butylcalix[4]arene (**1**) was attempted, under the very same general conditions used for the difunctional counterpart, huge amounts of dimeric, trimeric and oligomeric materials were obtained, whatever the particular conditions tested. We now report that a highly efficient polymerization of **1** has been accomplished by Rh-based ternary catalytic systems. In one case, the initiator was prepared *in situ* from $[\text{Rh}(\text{nbd})\text{Cl}]_2$, 1,1-diphenyl-2-phenylvinyl lithium (TPVLi) and PPh_3 in toluene, adapting a reported procedure by Masuda *et al.* for the living polymerization of monosubstituted phenylacetylenes (PA). After 1h at 30°C, monomer **1** was quantitatively con-

verted (GPC analysis) affording **poly 1** in high yield, with virtually no oligomeric materials. A second ternary catalytic system, firstly developed by Noyori *et al.* for PA, was similarly prepared, using $\text{PhC}\equiv\text{CLi}$ instead of TPVLi as the rhodium alkylating agent. It also proved effective in the polymerization of **1**, albeit in a less efficient way, requiring extended reaction times for complete conversion of the monomer and producing a polymer with a larger polydispersity under the conditions used. The underlying features of these polymerization systems will be reported.

BULK THERMAL POLYMERIZATION OF PHENYLETHYNYL-CALIX[4]ARENE COMPOUNDS

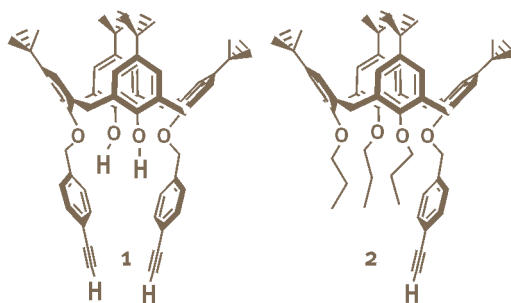
Barata, P.D.; Costa, A.I.; Prata, J.V.

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C. de Inv. de Engenharia Química e Biotecnologia, ISEL, Lisboa, Portugal

As part of an ongoing project aiming to study the polymerizabilities of calix[4]arene compounds having phenylethynyl groups appended at the calixarene lower rim, the bulk thermal polymerization of compounds **1** and **2** was studied. The bulk polymerization of **1** was undertaken in a sealed vessel under argon at 205°C (15 min.). Contrary to our initial expectations, the polymerization of **1** did not yield an insoluble polymer. Indeed, a completely soluble (THF) brownish-orange residue was obtained which contained less than 15% of starting **1**, 7% of dimer, 5% of trimer and 75% of a polymer from which a yellow

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polymer was isolated in 49% ($M_n = 570 \text{ gmol}^{-1}$; $M_w/M_n = 2.9$; GPC analysis). Its infra-red spectrum resembles that of a polymer obtained under Rh(I) catalyzed polymerization. In addition, a rather small ethynylic stretching frequency at 2110 cm^{-1} ($\text{-C}\equiv\text{C-}$) was also discernible, probably accounting for the linear dimeric/trimeric products (from Glaser and/or Strauss type couplings) found in the isolated polymer. Polymerization of **2** on the other hand did produce an insoluble material which, due to the monomer structure, could not result from direct cross-linking reactions. In order to better understand the polymerization processes involved, a TG/DSC study was performed. When heated under N_2 ($7^\circ\text{C}/\text{min}$) up to 230°C , the DSC thermogram of **1** shows an endothermic event peaking at 160°C which correspond to the melting of **1**, immediately followed by an exothermic transition

peaking at 186°C. This event corresponds to the thermal polymerization of melted **1**, for which an enthalpy of 110 10 kJmol⁻¹ was calculated. The GPC composition of the brownish-red residue thus obtained was very similar to that referred above. The DSC trace of **2** (when heated up to 255°C) shows the same observable trends as in the case of **1**, that is, an endothermic transition at 158°C (melt), followed by polymerization (peaking at 234°C) with an associated enthalpy of 220 kJmol⁻¹. Most of the residue (73%) was insoluble in THF which has an IR spectrum identical to the polymer obtained under catalysis. The dissimilar and unexpected behavior of calixarenes **1** and **2** as well as the main underlying mechanisms involved in their thermal induced reactions, will be discussed in this communication.

SATISFAÇÃO DO CLIENTE – CONCEITOS E MEDIÇÃO

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C. de Est. de Gestão, Inst. Sup. Técnico – Tagus Park, Porto Salvo, Portugal

Este seminário tem como finalidade apresentar os principais conceitos de satisfação do cliente bem como as principais metodologias que têm vindo a ser usadas nos últimos anos na sua avaliação. Faz-se uma análise crítica às escalas de medição e a sua influência nas técnicas de análise de dados. Apresenta-se uma nova metodologia para medição e análise da satisfação do cliente. O modelo matemático deriva da análise conjunta e expressa as relações fundamentais entre os critérios e a satisfação global. O procedimento usado para estimar o modelo baseia-se na regressão com variáveis mudas e com restrições. O método pode, de uma forma simples, usar dados não métricos através da codificação dos níveis dos critérios, sendo assim possível considerar os julgamentos qualitativos dos clientes. Recorrendo a um exemplo, interpretam-se os resultados com base nas funções de utilidade para cada critério e apresentam-se as principais vantagens do método.

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*Seminários CEG-IST,
Lisboa, 16 de Março
de 2007.*

BIOCATALYSIS OF *Coriolus Versicolor* BIOMASS CONTAINING GLUCOSE 2-OXIDASE ACTIVITY AT HIGH PRESSURES

Karmali, A.; Reis, E.; Henriques, C.; Coelho, J.

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DEQ, Lisbon, Portugal

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*Livro de abstracts of
5th International
Symposium on High
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Technology and
Chemical Engineering,
Segovia, 24 to 27 of
June of 2007.*

The present work involves the conversion of D-glucose into D-glucosone in the presence of *Coriolus versicolor* biomass at high pressures with compressed air in a modified commercial reactor. Several parameters affecting biocatalysis at high pressures, up to 20 MPa, were investigated as follows: temperature, pressure, pH, biomass concentration and glucose concentration. The data presented in this work strongly suggests that the rate of reaction increases with temperature, pressure and glucose concentration. The optimum temperature and pH for conversion of D-glucose into D-glucosone was 55°C and at pH 5.0, respectively. On the other hand, the kinetic constants (*i.e* Km and Vmax) were also determined at high pressure which was found to be 2.95mM and 8.8U/mg protein for Km and Vmax, respectively. The use of biomass containing glucose 2-oxidase activity was also useful for conversion of D-glucose into D-glucosone. Moreover, the re-utilization of biomass for this conversion at high pressure revealed that the yield was about 50%.

SUPERCRITICAL FLUID EXTRACTION, HYDRODISTILLATION AND SOXHLET EXTRACTION OF THE AERIAL PART OF WINTER SAVORY: COMPARATIVE EVALUATION OF THE EXTRACTION METHOD ON THE CHEMICAL COMPOSITION

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Supercritical fluid extraction of the volatile oil of the aerial part of the winter savory was carried out in different conditions of pressure, temperature, mean particle size and CO₂ flow rate and the results were compared with those obtaining by hydrodistillation with a Clevenger-type apparatus. The non-volatile components were extracted by SFE at higher pressures and by soxhlet extraction with different solvent mixtures. Concerning the volatile components, although the extraction yields of SFE and HD are quite similar, SFE extracts are richer in thymoquinone, a component with interest to the pharmaceutical industry due to its anti-cancer, antioxidant and anti-inflammatory properties.

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Livro de abstracts of European Congress of Chemical Engineering, Copenhagen, 16 e 20 of September of 2007.

HOW BIOMIMETICS SYNTHETIC HYDROXYAPATITE CAN BE?

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Materiais 2007,
Porto, 2007.

Hydroxiapatite (HAP) is a calcium phosphate with chemical composition similar to that of the mineral compound of natural bones, dental enamels and dentin. This bioceramic has been extensively used in orthopaedic, dental and maxillofacial applications to support bone ingrowths and osteointegration because it mimics the chemical composition and structure of natural bones showing, additionally, good biocompatibility with the human organism. Over the last few years, a number of novel processes for preparing HAP powders have been developed. The stoichiometry, the crystallite size and thermal stability of synthesized HAPs are properties that need a special control during the manufacturing. In the present work, natural bone (cortical and spongy) and different synthetic HAPs have been compared. The synthetic powders were previously characterized using chemical analysis, surface area measurements, laser diffraction, mercury porosimetry, X-ray diffraction (XRD), simultaneous thermogravimetry/differential thermal analysis (TG-DTG/DTA) and field emission gun-scanning electron microscopy FEG-SEM as well as electron transmission electron microscopy (TEM). The synthetic powders are thermally stable up to 1000°C and the thermogravimetric curves show a mass loss in two-stages, ranging between 8 and 10%. Almost all the properties investigated revealed a dependency on the nature of the powders. In order to compare the mechanical properties of synthetic HAPs with those of natural bone an explosive compaction/consolidation process of the encapsulated powders of both origins (synthetic and natural), has been carried out. Recently it has been demonstrated that powders can be consolidated with shock waves in appropriate pressure ranges and durations depending on the SSS powders characteristics (Structure, Shape and Size distribution). The pressures in the shock front that moves through the powders can overcome their flow stress (GPa) and powders near the surface can attain temperatures high enough to induce the fusion temperature of the material. However, due to the instantaneous character of this phenomenon, the time is not sufficient to change the original micro- and nanostructure. Besides density of encapsulated powders, pressure and pulse dura-

tion are variable, that can play an important role in the control of porosity of HAPs. Optical and electron scanning microscopies were used to examine pores and cracks size distribution. X-ray diffraction and TEM revealed that all the samples exhibit nanosized crystallites. The mechanical properties (hardness, Young's modulus and Yield stress) of the compacted samples with different degrees of porosity were compared using the values resulting from depth sensing indentation technique and the new reverse analysis method, that was successful tested in the presumption of mechanical properties of single and bi-phase materials.

ESTRATÉGIAS E TECNOLOGIAS MAIS ADEQUADAS PARA O TRATAMENTO DE RESÍDUOS SÓLIDOS COM VALORIZAÇÃO ENERGÉTICA

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Engenharias 07,
Covilhã, 2007.*

Neste artigo, pretende-se abordar as estratégias de gestão de resíduos sólidos, à luz da legislação nacional e comunitária nesta matéria, bem como as melhores tecnologias aplicadas às mais importantes fileiras de resíduos, nomeadamente, urbanos e industriais, perigosos e banais. As várias opções tecnológicas para o tratamento por valorização ou eliminação de resíduos, assenta em variadas vertentes, nomeadamente, de viabilidade técnica e funcional, legal, económica e, por último, mas não menos importante, ambiental. Um dos objectivos deste artigo, é comparar as várias tecnologias competitivas entre si, nomeadamente, através das mais-valias ambientais e energéticas obtidas. É possível concluir, por exemplo, que, face às imposições legais comunitárias em matéria de reciclagem de resíduos e de minimização da utilização de aterros, está aberta uma grande janela de oportunidade para o desenvolvimento dos métodos biológicos com valorização material/energética, como a Compostagem e a Digestão Anaeróbia, para tratamento dos resíduos de fracção orgânica biodegradável. Os métodos de incineração aplicam-se essencialmente aos resíduos perigosos e que não possam ser sujeitos a outras alternativas de tratamento.

LEVELS OF LEAD AND CADMIUM CONTAMINATION IN CABBAGE BY ASV AND GFAAS

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Contamination by heavy metals is indeed widespread all over the world and their presence occurs in both natural and anthropogenic forms. While usually natural forms are present at relative low concentrations, in recent years a number of anthropogenic sources such as vehicle exhausts, waste incineration, metal processing, dumping of waste, fertilizers and agricultural waste, have implied notable contributions to the increase of environmental metal concentrations.

As a result of the increase of this contamination, governments of most developed and industrialized countries have modified their legislations in order to minimize the environmental levels of these elements. The abolition of leaded gasoline has implied an important reduction of the levels of lead into the environment. In Lisbon our group has confirmed this fact by measuring lead levels in *populus* leaves, used as bioindicator. But the levels of lead and cadmium in Lisbon soils remain very high as we have confirmed. This high levels of lead accumulated throughout several years and the continuous emissions of this metal by the automobile traffic (nowadays in much lowers quantities, but the gasoline still has a reasonable amount of lead) that are deposited in the proximity of the roads reveals an environmental problem. In Lisbon there is a reasonable amount of small vegetable plots in the surrounding of roads of high traffic intensity. In this vegetable plots are produced cabbage and other vegetables that are used for human nourishment and are seen as organic food because there is no use of fertilizers. In this study we have measured the lead and cadmium levels of cabbage cultivated in this vegetable plots near high traffic roads.

Leaves of traditional cabbages were collected and immediately dried in an oven at 60°C during two days to lose completely their water content. Afterwards, the dried cabbage was crushed in an agate ball mill until reduced to a fine powder. The powder was digested in a traditional way with nitric acid and hydrogen peroxide from Merck (Suprapur grade). The cadmium and lead in the samples were determined by ASV (Anodic Stripping Voltammetry) and GFAAS (Graphite Furnace Atomic Absorption Spectrometry).

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The preliminary values of lead contamination in some locals of Lisbon are shown below. The values obtained by both methods are similar and reveal a reasonable lead contamination in the cabbages.

Local	[Pb] (mg/mg of dry matter)	
	GFAAS	ASV
#1	0.258	0.305
#2	0.158	0.269
#3	0.153	0.183

The cadmium determination is under way. The attempts to realize the digestion process of these samples by microwave technology have failed due to the violent interaction of the cabbage powder when exposed to micro-

wave radiation. Also a PTFE reactor has been destroyed in this process. These facts will be investigated by us and by CEM Corporation (the manufacturer of our microwave reactor).

RELATIONSHIPS BETWEEN Cu AND Ni CONTENT AND PHYSICO-CHEMICAL PROPERTIES OF SOILS IRRIGATED WITH WASTEWATER

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Reuse of wastewaters plays an important role in the management of water resources, which is particularly relevant in the Mediterranean Region where demand increases while quality tends to decrease. Use in agriculture takes the benefit from and contributes to recycling of nutrients and water. However, high contents in toxic and phytotoxic metals present in the water added to the soil, may promote negative effects.

This research study has been conducted to evaluate the relationship between the accumulation of metals in soils and some physical and chemical properties of soils (Leptosols, LPs, and Cambisols, CMd) irrigated with untreated wastewater, secondary treated wastewater or normally used groundwater.

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DETERMINAÇÃO DE METAIS TÓXICOS NUMA MATRIZ ALIMENTAR POR SWASV: ELÉCTRODO DE FILME DE MERCÚRIO vs. ELÉCTRODO DE FILME DE BISMUTO

**Silva, Nelson A.F.; Silva, Hugo F.A.;
Oliveira, Sandrina; Galego, Pedro; Matos, Manuel J.**

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X Iberic Meeting of
Electrochemistry and
XIV Encontro da
Sociedade Portuguesa
de Electroquímica,
Coimbra, 12 a 14 de
Abril de 2007.*

O risco de consumirmos alimentos contaminados é um problema cada vez mais actual exigindo o recurso a procedimentos de conservação, processamento, distribuição e controlo de qualidade nutricional e toxicológicos cada vez mais rigorosos. Este problema torna-se bastante mais preocupante quando o circuito de determinados alimentos se processa desrespeitando os procedimentos legais, podendo daí advir consequências graves, em termos de saúde, para o consumidor final. Um exemplo que elucida esta situação prende-se com a existência de pequenas áreas de exploração agrícola (hortas) nas bermas e taludes das vias de tráfego automóvel intenso. De facto, esta prática é cada vez mais frequente, com os géneros alimentícios tipicamente existentes a serem cultivados em zonas altamente poluídas, sendo posteriormente alvo de comercialização e consumo humano sem qualquer controlo de qualidade.

O presente trabalho consiste num estudo de caracterização da contaminação de folhas de couve galegas (*Brassica oleracea*, grupo *Acephala*), por metais tóxicos, recolhidas em hortas situadas na berma das principais vias de tráfego automóvel de Lisboa. A técnica utilizada nestas determinações foi a Voltametria de Redissolução Anódica de Onda Quadrada (SWASV), a qual se caracteriza por ser uma técnica rápida, de baixo custo, possibilidade de determinação simultânea de vários metais, baixo limite de detecção e possibilidade de efectuar análises *in situ*. Os metais estudados foram o cádmio e o chumbo.

Foram realizados ensaios das várias amostras com um eléctrodo de filme de mercúrio, tradicionalmente utilizado neste tipo de análises, e com um eléctrodo de filme de bismuto. O bismuto é um material de eléctrodo que recentemente surgiu como forte alternativa à utilização de mercúrio em electroanálise, em função da toxicidade deste último. Foram analisados os resultados e comparadas as performances electroanalíticas de cada eléctrodo. Estes mostram de facto um comportamento bastante idêntico entre ambos os eléctrodos pelo que somos da opinião que o eléctrodo de filme de bismuto é uma alternativa válida à utilização do eléctrodo de filme de mercúrio na determinação

simultânea de metais tóxicos em amostras reais de matriz complexa por Voltametria de Redissolução Anódica de Onda Quadrada (SWASV). Os resultados mostram também a presença de níveis razoáveis de metais tóxicos nestes legumes. Os seus teores poderão originar diversas doenças graves como é referido em Ravindra, 2004. Será assim de desencorajar a existência de zonas de cultivo próximas de vias de elevado volume de tráfego automóvel, sejam estas de índole particular, ou fazendo parte de unidades de produção agrícola.

CHEMISTRY IN AQUEOUS MEDIUM AT THE IST GROUP: AN OVERALL VIEW

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Publicado em:
*Livro de Abstracts do
3rd Annual AQUACHEM
Meeting, Debrecen,
Hungria, Janeiro de
2007.*

During the third year of the AQUACHEM Project, the studies of the IST group were mainly directed towards the following areas:

I syntheses of metal complexes with water soluble phosphines, namely the first examples of copper complexes bearing tpa or any derived ligand with a cage-like tpa core, and Pt(II or IV) complexes;

I syntheses of iron complexes with the “N₂S₂” ligand and study of their catalytic activity in the peroxidative oxidation of cyclohexane;

I synthesis of copper(II)-aminopolyalcoholbenzenepolycarboxylate coordination polymers;

I application of water soluble mono-, di- and polynuclear copper complexes as catalysts for the peroxidative oxidation of alkanes under mild conditions;

I functionalization of hydrotris(1-pyrazolyl)methane providing different classes of new ligands;

I syntheses of metal complexes with water soluble scorpionate ligands and their application as catalysts for the oxidation of alkanes under mild conditions;

I study different applications of trispyrazolyl ligands in the chemistry of dendrimers;

I application of Pt-PTA and Re complexes in the Baeyer-Villiger oxidation reactions;

I electrochemical investigation of water soluble metal complexes.

These studies are outlined and their significance from synthetic, catalytic and biological viewpoints is discussed.

WATER-SOLUBLE SCORPIONATES OF RHENIUM AND IRON

Alegria, E.^{1,2}; Martins, L.^{1,2}; Pombeiro, A.²

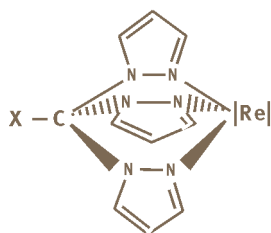
1 Departamento de Engenharia Química, ISEL, Lisboa, Portugal

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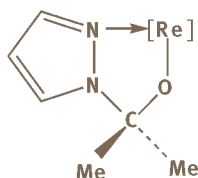
The coordination chemistry of “scorpionate” nitrogen donor ligands has been widely developed in the last years and their complexes have found applications in processes with biological and industrial significance.

We now report the reactions of HCpz_3 and $\text{Li}[\text{SO}_3\text{Cpz}_3]$ with Re and Fe centres, leading to the first tris(pyrazolyl)methanesulfonate complexes of rhenium(V and VII) and iron(II) and to some hydrotris(pyrazolyl)methane complexes of these metals. In addition, an unusual acetone-pyrazolyl coupling led to a chelated pyrazolyl-alkoxide.

Their redox properties, studied by cyclic voltammetry, allowed to estimate, for the first time, the Lever electrochemical E_L parameter for the $\text{SO}_3\text{C}(\text{pz})_3$ - and oxo ligands.



X = SO_3^- , H



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The catalytic activity of some complexes in the peroxidative oxidation of cyclohexane to the corresponding alcohol and ketone, under mild conditions, in aqueous medium and with an environmentally friendly oxidant is also reported.

SYNTHESIS AND REACTIONS OF SCORPIONATES: COORDINATION TO FE AND COUPLING WITH A DENDRIMER

Wanke, R.¹; Alegria, E.^{1,2}; Servin, P.³; Smolenski, P.¹; Martins, L.^{1,2}; Caminade, A.-M.³; Pombeiro, A.¹

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 3rd Annual AQUACHEM
 Meeting, Debrecen,
 Hungria, Janeiro de
 2007.*

The coordination chemistry of tridentate nitrogen donor ligands has been quite developed in the last years namely due to the applications of their complexes in industrial and biological processes. In pursuit of our interest on the coordination chemistry of the N₃ tripodal neutral hydrotris(1-pyrazolyl)methane (HCp₃, Tpm) and its reactions with iron (II) centres,² we have been investigating some functionalization reactions of HCp₃ and coordination and coupling reactions of such species. We now report the reactions of scorpionate iron(II) complexes, e.g., [FeCl₂(HCp₃)] or [FeCl₂(SO₃Cp₃)] with PTA (1,3,5-triaza-7-phosphaadamantane) or derivatives, which are water soluble phosphines. We also report the reactions of FeCl₂·2H₂O with the above phosphines leading to complexes of type [FeCl₂(PTA)_n], that can further react with Tpm. Attempts to increase the water solubility of this type of complexes will also be discussed. Their synthesis and characterization by IR and multinuclear NMR spectroscopies, FAB⁺-MS spectrometry, elemental analysis and electrochemical methods are also presented. With the cooperation of the Toulouse group, we have coupled HO-CH₂-Cp₃ with G_{cl} dendrimer bearing -CH₂I on the surface. Other coupling approaches will be reported by P. Servin.

TRIS(1-PYRAZOLYL) METHANESULFONATE VANADIUM(IV) COMPLEX, A WATER-SOLUBLE CATALYST FOR OXIDATION OF ALKANES

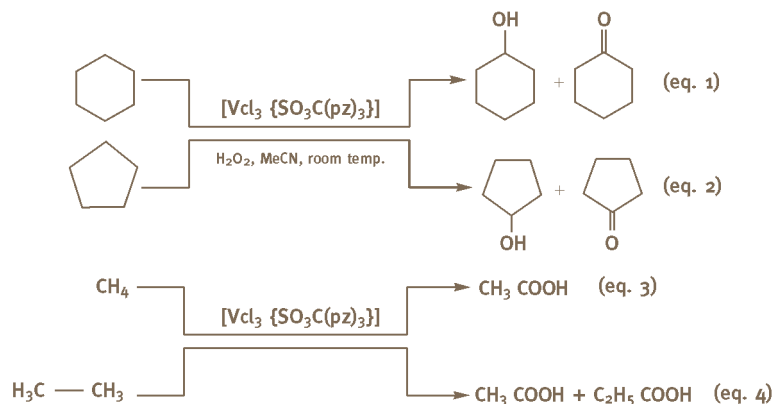
Silva, Telma F.S.^{1,3}; Martins, Luísa M.D.R.S.^{2,3};
Pombeiro, Armando J.L.³

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In the attempt to develop new processes for a more sustainable chemistry, we have been able to synthesise a V(IV) complex with the tris(1-pyrazolyl)methanesulfonate ligand, $[\text{VCl}_3\{\text{SO}_3\text{C}(\text{pz})_3\}]$, which is water-soluble and acts as a catalyst, or catalyst precursor, under mild conditions, in the peroxidative oxidation of cyclohexane (eq. 1) or cyclopentane (eq. 2) into their corresponding alcohols and ketones in aqueous/acetonitrile medium; as well as in the oxidation of methane or ethane to acetic and/or propionic acid, in a single-pot process, in the presence of the peroxodisulfate salt $\text{K}_2\text{S}_2\text{O}_8$ as the oxidizing agent and in trifluoroacetic acid as the solvent (eqs. 3 and 4).

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Meeting, Debrecen,
Hungria, Janeiro de
2007.*



Reaction conditions, turnover numbers and yields are reported.

ELECTROCHEMICAL BEHAVIOUR OF NEW SCORPIONATE OXO-VANADIUM COMPLEXES

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 de Electroquímica,
 Coimbra, Portugal,
 Abril de 2007.*

Vanadium scorpionate complexes have received attention as possible models for the bonding of vanadium in biomolecules in particular vanadoenzymes. The scorpionate ligands have a number of attractive features and provide suitable systems for study of the structural, redox and mechanistic possibilities available to vanadium in bioinorganic systems.

However oxovanadium complexes containing the scorpionate ligands have not yet been the object of an electrochemical investigation.

We now report the results of our study of the electrochemical behaviour of new oxovanadium complexes, obtained by reaction of VO(OEt)₃ with HB(pz)₃, HB(3,5-Me₂pz)₃, HC(pz)₃, HC(3,5-Me₂pz)₃ and Li[SO₃C(pz)₃], carried out in 0.2 M [Bu₄N][BF₄]/CH₂Cl₂, by cyclic voltammetry (CV) at a Pt-disc electrode and by controlled potential electrolysis (CPE) at a Pt-gauze electrode.

The obtained electrochemical results are discussed in terms of electron richness of the vanadium centres, the electronic properties of the scorpionate ligands and are compared with related complexes in literature.

ELECTROCHEMICAL STUDY OF RU(II)-CYMENE COMPLEXES

Wanke, Riccardo¹; Kuznetsov, Maxim L.¹;
Martins, Luísa M.D.R.S.^{1,2}; Pombeiro, Armando J.L.¹;
Marchetti, Fabio³; Pettinari, Claudio³;
Pettinari, Riccardo³; Cerquetella, Adele³;
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Half-sandwich η^6 -arene-ruthenium compounds are important in catalysis and a further recent interest stems from the synthesis of water-soluble examples which exhibit antibiotic and antiviral activities.¹

We have now investigated the electrochemical behaviour of a series of complexes of formulae I and II (Fig. 1) derived from (cymene)ruthenium(II) dichloride.

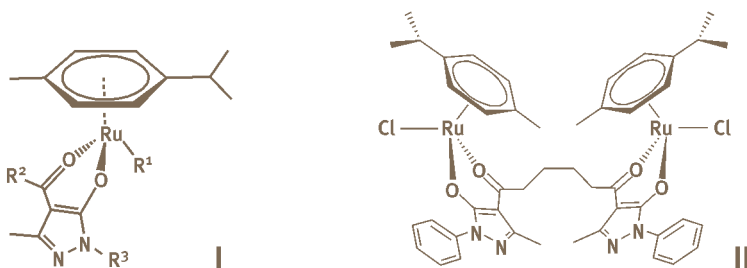


Figure 1. R = Cl-, N₃⁻, PPh₃

Their redox properties have been studied by cyclic voltammetry and controlled potential electrolysis, at a Pt electrode, in a 0.2M [ⁿBu₄N][BF₄]/CH₂Cl₂ solution, at 25°C.

They exhibit a single-electron (per metal atom) reversible oxidation, assigned to the Ru^{II} → Ru^{III} oxidation, at the half-wave oxidation potential values in the ranges 1.25-1.57 and 1.55-1.63 V vs. SCE for the neutral and cationic complexes, respectively.

These results have allowed to order the acylpyrazolonate ligands according to their electron-donor character but indicate a limited variation of the HOMO energy upon change of the ligand R¹. Implications on the HOMO composition are discussed.

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ELECTROCHEMICAL BEHAVIOUR OF OXORHENIUM(V) COMPLEXES WITH *N,O*-LIGANDS

Granada, Margarida C.¹; Alegria, Elisabete C.B.^{1,2};
Kirillov, Alexander M.²; Martins, Luísa M.D.R.S.^{1,2};
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Encontro da
Sociedade Portuguesa
de Electroquímica,
Coimbra, Portugal,
Abril de 2007.*

The oxo chemistry of rhenium is attracting much interest, in particular due to the discovery that $[(\text{Me})\text{ReO}_3]$ and its derivatives are among the most versatile oxidation catalysts.^{1,2} Nevertheless, the application of inorganic coordination compounds of rhenium in catalysis remains little explored, namely in the functionalization of alkanes.

Recently we have prepared³ from $[\text{ReOCl}_3(\text{PPh}_3)_2]$ precursor a series of oxorhenium(V) complexes (Fig. 1) derived from *N,N*-bis(2-hydroxyethyl) glycine (bicine) (1), *N*-(2-hydroxyethyl)iminodiacetic (2), picolinic (3) or dipicolinic (4) acids, which have been found to exhibit a remarkable catalytic activity for the carboxylation of ethane by CO, in a single pot process and under mild conditions, to give propionic acid as a main product.

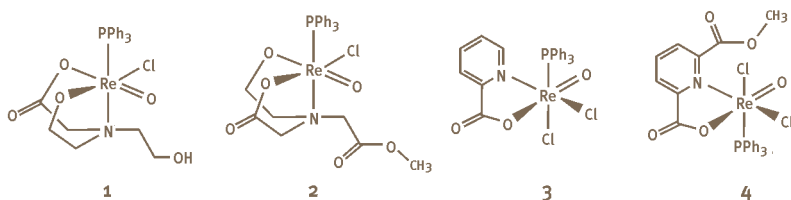


Figure 1.

Herein we report the results of electrochemical study of these oxorhenium(V) compounds by cyclic voltammetry (CV) and controlled potential electrolysis (CPE), in 0.2M $[\text{NBu}_4][\text{BF}_4]$ / CH_2Cl_2 and at room temperature, using the Pt-wire or -gauze electrodes, respectively. The obtained electrochemical results are discussed in terms of electron properties of the rhenium centres and the ligands.

ELECTROCHEMICAL BEHAVIOUR OF BENZOYL-HYDRAZIDO AND -DIAZENIDO RHENIUM COMPLEXES WITH CHELATING *N,O*-LIGANDS

Reis, Telma C.¹; Alegria, Elisabete C.B.^{1,2};
Kirillov, Alexander M.²; Martins, Luísa M.D.R.S.^{1,2};
Pombeiro, Armando J.L.²

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The benzoylhydrazido complex $[\text{ReCl}_2\{\text{MNC}(\text{O})\text{Ph}\}(\text{PPh}_3)_2]$ is a key starting material for the synthesis of a variety of rhenium compounds with significance in the fields of nuclear-medical research, nitrogen fixation or catalysis. However, its use for the synthesis of diazenido and dinitrogen complexes with *N*-coligands is still very rare and usually limited to amines. We were able to extend the application of the above precursor to the synthesis of benzoyl-hydrazido Re(V) and - diazenido Re(III) complexes **1-5** (Fig. 1) with various *N,O*-coligands,¹ such as triethanolamine (**1**), *N,N*-bis(2-hydroxyethyl)glycine (**2**), *N*-hydroxyimino-diacetic (**3**), *N*-hydroxy-2,2'-iminodipropionic (**4**) and picolinic acids (**5**), or their derived forms.

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Livro de Abstracts do IX Encontro Ibérico de Electroquímica e XIV Encontro da Sociedade Portuguesa de Electroquímica, Coimbra, Portugal, Abril de 2007.

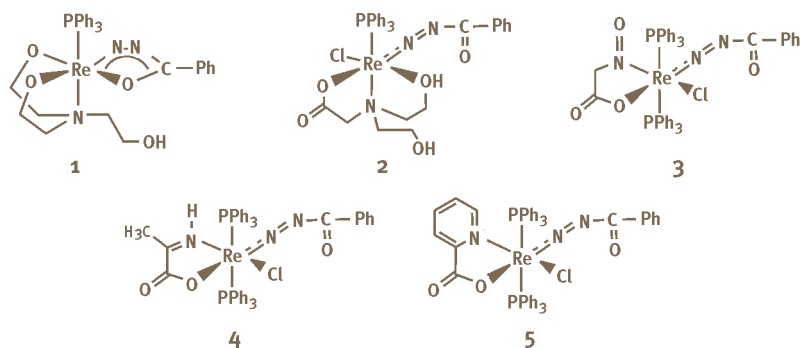


Figure 1.

We now report the study of the electrochemical behaviour, by cyclic voltammetry (at a Pt-disc electrode) and by controlled potential electrolysis (at a Pt-gauze electrode), of the above benzoyl-hydrazido and -diazenido rhenium complexes (Fig. 1) with chelating *N,O*-ligands. The obtained electrochemical results are discussed in terms of electron richness of the Re(V) (**1**) and Re(III) (**2-5**) centres and the electronic properties of the ligands.

SCORPIONATE RHENIUM COMPLEXES AS CATALYSTS FOR THE BAEYER – VILLIGER OXIDATION WITH AQUEOUS H_2O_2

Travassos, Catarina¹; Alegria, Elisabete C.B.^{1,2}; Martins, Luísa M.D.R.S.^{1,2}; Pombeiro, Armando J.L.²

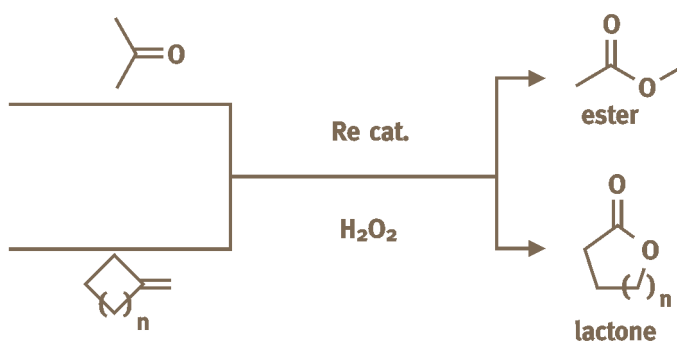
¹ Departamento de Engenharia Química, ISEL, Lisboa, Portugal

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 Livro de Abstracts do
 3rd International
 Conference on Green
 and Sustainable
 Chemistry, University
 of Delft, Holanda,
 Julho de 2007.

Recently, we have found that the pyrazole $[ReCl_2\{N_2C(O)Ph\}(Hpz)(PPh_3)_2]$ ($Hpz = \text{pyrazole}$), $[ReCl_2\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ and $[ReCl\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$, the tris(pyrazolyl)methane $[ReCl_2(HCpz_3)(PPh_3)]$ $[BF_4]$ ($pz = \text{pyrazolyl}$), $[ReCl_3(HCpz_3)]$ and the tris(pyrazolyl)methanesulfonate $[ReOCl_2(SO_3Cpz_3)(PPh_3)]$ and $[ReO_3(SO_3Cpz_3)]$ compounds, as well as their precursors $[ReCl_2\{\eta^2-N,O-N_2C(O)Ph\}(PPh_3)_2]$ and $[ReOCl_3(PPh_3)_2]$, act as selective catalysts (or catalyst precursors), in the single-pot oxidation of ethane to acetic acid and in the peroxidative oxidation of cyclohexane to cyclohexanone and cyclohexanol. As an extension of the latter studies, we now report the application of the above scorpionate rhenium complexes as catalysts for the Baeyer-Villiger oxidation of cyclic and acyclic ketones to the corresponding lactones or esters, by an aqueous diluted solution of H_2O_2 , a green oxidant, under mild conditions.

The effects of various parameters such as the amount of catalyst, type of oxidant or solvent, reaction time or temperature were investigated.



UNPRECEDENTED USE OF MICROWAVES IN THE SYNTHESIS OF SCORPIONATE AND DERIVED PYRAZOLE RHENIUM COMPLEXES

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Recently, we have been able to synthesise and characterize a series of rhenium complexes with the hydrotris(1-pyrazolyl)methane (*e.g.*, $[\text{ReCl}_2(\text{HCpz}_3)(\text{PPh}_3)]\text{[BF}_4\text{]}$ or $[\text{ReCl}_3(\text{HCpz}_3)]$), the tris(1-pyrazolyl)methanesulfonate (*e.g.*, $[\text{ReOCl}_2(\text{SO}_3\text{Cpz}_3)(\text{PPh}_3)]$ or $[\text{ReO}_3(\text{SO}_3\text{Cpz}_3)]$), and with the related pyrazole (*e.g.*, $[\text{ReClF}\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})(\text{PPh}_3)_2]$ (Hpz = pyrazole)) ligands, and we have found that they act as selective catalysts, in the single-pot oxidation of ethane to acetic acid and in the peroxidative oxidation of cyclohexane to cyclohexanone and cyclohexanol. However, their syntheses often require an inconvenient reflux during several hours or days, what has encouraged us to try to improve the synthetic method.

Herein we report a convenient microwave-assisted synthesis of the above rhenium complexes which, by taking advantage of this alternative and efficient source of energy, greatly shortens the reaction times (from days to a few minutes) and the amount of solvent used, and leads to improved product yields. The effects of reaction conditions (*e.g.*, temperature and pressure) are also indicated.

Publicado em:

Livro de Abstracts do 41st IUPAC World Chemistry Congress, Lingotto Conference Centre of Turin, Itália, Agosto de 2007.

SYNTHESIS AND COORDINATION OF NEW SCORPIONATES

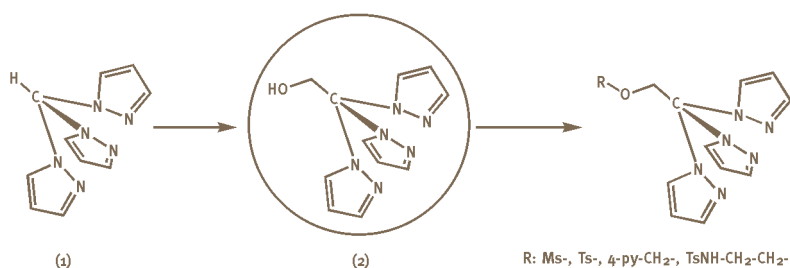
Wanke, R.¹; Martins, L.^{1,2}; Pombeiro, A.J.L.¹

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Publicado em:
*Livro de Abstracts do
 XVII EuCheMS
 Conference on
 Organometallic
 Chemistry, Sofia,
 Bulgária, Setembro de
 2007.*

The coordination chemistry of tridentate nitrogen donor ligands has been developed in the last years namely due to the application of their complexes in industrial and biological processes. However, in contrast to the widely studied anionic hydrotris(1-pyrazolyl)borate (HBpz₃, Tp; pz: pyrazolyl), the coordination of the isoelectronic N₃ tripodal neutral hydrotris(1-pyrazolyl)methane (HCpz₃, Tpm) and its derivatives has been much less investigated and still constitutes an underdeveloped field of research.

In this work, we present the synthesis of new derivatives of Tpm and their coordination to several metal centres. In fact, HCpz₃ (1, Scheme 1), has been functionalized to prepare the derivative tris-2,2,2-(1-pyrazolyl)ethanol (2) which shows interesting properties of solubility and reactivity for further functionalization. Starting from 2, we were able to synthesize several new tris(1-pyrazolyl) compounds, fully characterize them and study their features such as solubility and coordination properties to Fe(II), Cu(I) and Co(II) centres.



Scheme 1.

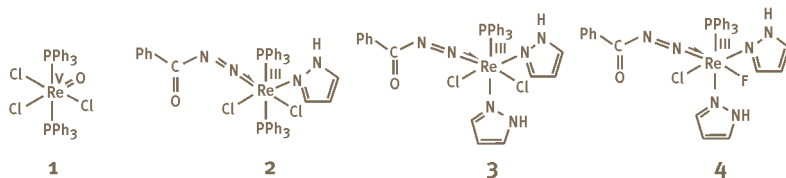
EFFECTIVE OXYFUNCTIONIZATION OF N-HEXANE WITH MOLECULAR OXYGEN CATALYZED BY SOLUBLE AND SUPPORTED RHENIUM COMPLEXES

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Martins, Luísa R.^{1,2}; Pombeiro, Armando J.L.¹

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Within our interest on the oxidative functionalization of alkanes under mild conditions, we have applied some Re complexes (**1-4**) supported on 3-aminopropyl functionalized silica for the catalytic oxidation of n-hexane, a cheap and easily available compound, whom functionalization by oxidation with O₂ has gained a considerable attention.



These supported rhenium complexes serve as effective catalysts for n-hexane oxidation in the presence of molecular oxygen without any additive, their activity being higher than that of the unsupported complexes in homogeneous system. The supported [ReClF{N₂C(O)Ph}(Hpz)₂(PPh₃)] **4** complex provides the best conversion (13%) and good selectivity towards ketone and alcohol derivatives of n-hexane. Some carboxylic acids were used as co-catalysts (2-pyrazinecarboxylic acid was the best found promoter). The reaction occurs under relatively mild conditions (150°C, 13.6 atm p(O₂) for 8h). Some evidences are presented in favour of the involvement of a free-radical mechanism. TGA analysis shows that the supported catalysts are stable up to reaction temperature.

Publicado em:

Livro de Abstracts do VIII International Symposium on Catalysis Applied to Fine Chemicals, Palianza - VB, Itália, Setembro de 2007.

MICROWAVE-PROMOTED PEROXIDATIVE OXIDATION OF ALKANES BAEYER-VILLIGER OXIDATION OF KETONES CATALYSED BY SCORPIONATE RHENIUM COMPLEXES

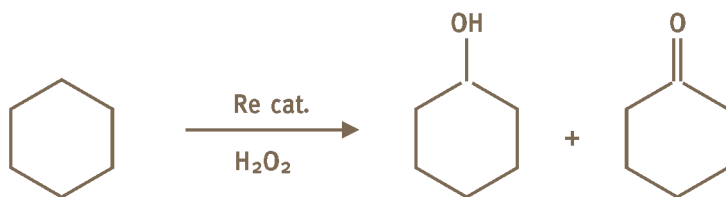
Furtado, Arlinda S.¹; Travassos, Catarina¹;
Alegria, Elisabete C.B.^{1,2}; Martins, Luísa M.D.R.S.^{1,2};
Pombeiro, Armando J.L.²

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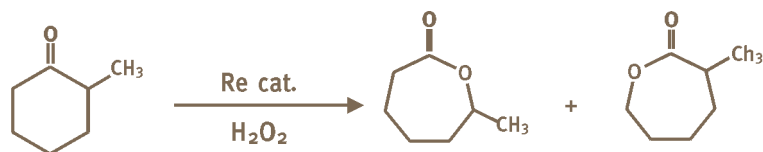
Publicado em:
*Livro de Abstracts do
8º Encontro da
Divisão de Catálise e
Materiais Porosos da
Sociedade Portuguesa
de Química, Lamego,
Portugal, Setembro de
2007.*

Scorpionate rhenium complexes act as selective catalysts (or catalyst precursors) for the peroxidative oxidation of cyclohexane to cyclohexanone and cyclohexanol and the Baeyer-Villiger oxidation of cyclic ketones to lactones, using an aqueous solution of H_2O_2 . The effects of a variety of factors were studied towards the optimization of the processes. These reactions are accelerated by microwave radiation that leads to an improved synthetic method which shortens the reaction time and increases the products yields. In pursuit of our interest on the coordination chemistry of the “scorpionate” nitrogen donor ligands, in particular of the N_3 tripodal neutral hydrotris(1-pyrazolyl) methane ($\text{HC}(\text{pz})_3$, Tpm) and the C-substituted sulfonate derivative tris (pyrazolyl)methanesulfonate ($\text{SO}_3\text{C}(\text{pz})_3$, Tpm_s) we have recently been able to synthesise and characterize a series of rhenium complexes with Tpm (e.g., $[\text{ReCl}_3(\text{HCp}_3)]$), Tpm_s (e.g., $[\text{ReO}_3(\text{SO}_3\text{Cp}_3)]$), and related pyrazole (e.g., $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})_2]$ (Hpz = pyrazole)) ligands. We have also found that they act as selective catalysts (or catalyst precursors) for the single-pot peroxidative oxidation of cyclohexane to cyclohexanone and cyclohexanol (Scheme 1).



Scheme 1. Peroxidative oxidation of cyclohexane to cyclohexanone and cyclohexanol.

Such complexes can also catalyse the Baeyer-Villiger oxidation of cyclic (Scheme 2) and acyclic ketones to the corresponding lactones or esters, by an aqueous diluted solution of H_2O_2 , under mild conditions.



Scheme 2. Baeyer-Villiger oxidation of 2-methyl cyclohexanone

The catalytic systems are based on the Re complexes **1-3** (Figure 1) in the presence of H_2O_2 as the oxidizing agent, in acetonitrile/water (Scheme 1) or 1,2-dichloroethane/water (Scheme 2) as the solvent, at room temperature (Scheme 1) or 70°C (Scheme 2) and a reaction time of 6 (Scheme 1) or 24 hours (Scheme 2).

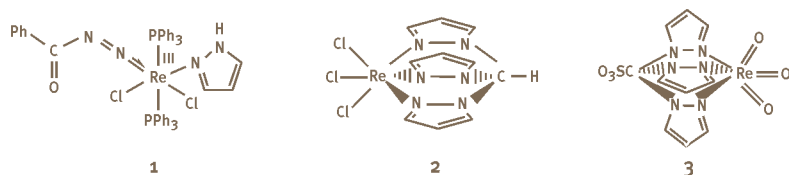


Figure 1.

Complex **1**, $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})(\text{PPh}_3)_2]$, provides the most active catalyst, which can give a conversion based on substrate over 90% being followed by complex **3**, $[\text{ReO}_3(\text{SO}_3\text{Cp}_2)]$.

MESOPOROUS SILICA SUPPORTED RHENIUM CATALYSTS FOR DIRECT OXIDATION OF N-HEPTANE BY MOLECULAR OXYGEN

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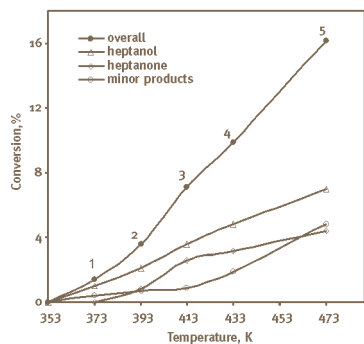
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*Livro de Abstracts do
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 Materiais Porosos da
 Sociedade Portuguesa
 de Química, Lamego,
 Portugal, Setembro de
 2007.*

Supported rhenium complexes serve as effective catalysts for n-heptane oxidation in the presence of molecular oxygen without any additive, their activity being higher than that of the unsupported complexes in homogeneous system. The supported $[\text{ReClF}\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})_2(\text{PPh}_3)]$ **4** complex provides the best conversion (10%) and good selectivity towards ketone and alcohol derivatives of n-heptane and 2-pyrazinecarboxylic acid works as a promoter. TGA analysis shows that the supported catalysts are stable up to reaction temperature.

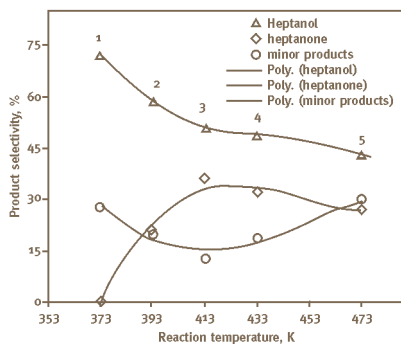
In the oxidation of hydrocarbons using dioxygen, one generally faces the following two problems. In addition, hydrocarbons do not have orbital of sufficiently high energy, accessible for chemical reaction and normally they required either very reactive oxidizing agents or extreme reaction conditions or both. For hydrogen peroxide as oxidizing agent several experiments of oxidation of alkanes using solid catalyst have been reported, but there are only few reported for dioxygen as the oxidizing agent. Heptane has been subjected to cracking (catalytic, homogenous or steam pyrolysis) to give mostly alkenes such as ethylene, propylene and butylenes. These processes require high temperature and calcium oxide supported over alumina ($\text{CaO}/\text{Al}_2\text{O}_3$) is one of the common catalysts which lower the reaction temperature and suppresses the coking formation. On using zeolite catalyst, the selectivity of a given alkane formation has been increased. In presence of O_2 using zeolite catalyst, the heptane was found to undergo partial oxidation along with cyclization from heptanone and heterocyclic compounds and others e.g. 2,3- and 4-heptanones, 2-methyl 5-ethylfuran, 2,6-dimethyl-pyran, 1-heten 4-ol and two branch dienes.

We are presenting here, some pyrazol rhenium complexes, $[\text{ReCl}_2\{\text{NNC}(\text{O})\text{C}_6\text{H}_5\}(\text{Hpz})(\text{PPh}_3)_2]$ (1), $[\text{ReCl}_2\{\text{NNC}(\text{O})\text{C}_6\text{H}_5\}(\text{Hpz})_2(\text{PPh}_3)_2]$ (2), and $[\text{ReClF}\{\text{NNC}(\text{O})\text{C}_6\text{H}_5\}(\text{Hpz})_2(\text{PPh}_3)]$ (3), which are analogue support on 3-aminopropyl functionalized mesoporous silica as a supported catalysts. These are act as efficient and selective heterogeneous catalysts for n-heptane oxidation, by O_2 , without requiring the any additives. The formed products by are mainly alcohols and ketones (4: 6 ratio), under low temperature and low pressure for very less reaction period.



Oxidation reaction by supported catalyst 4

Figure 1.



Product selectivity of n-heptane by supported catalyst 4

Figure 2.

The systems thus prepared behave as heterogeneous catalysts for the oxidation of n-heptane (3mL) by molecular oxygen under relatively moderate reaction conditions (393K, $p(\text{O}_2) = 10 \text{ atm}$) in batch reactor (22mL). The pyrazol rhenium complexes exhibits the good activity and product selectivity, which is further promoted by using 2-pyrazinecarboxylic acid as a co-catalyst, while picolinic acid proved to be almost inactive. Heptanol is the main product, whereas heptanone is formed in less amounts and other miner products are formed (Fig. 1 and 2). TGA analysis of the catalyst shows that it is stable at the reaction temperature and inductive couple plasma analysis indicates a negligible metal loss upon 20h use of the catalyst up to 150°C reaction temperature.

USE OF MICROWAVES TO GET SCORPIONATE VANADIUM AND RHENIUM COMPLEXES

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Alegria, Elisabete C.B.A.^{2,3};
Martins, Luísa M.D.R.S.^{2,3}; Pombeiro, Armando J.L.³**

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The scorpionate ligands have a number of attractive features and provide suitable systems with vanadium and rhenium in bioinorganic and catalytic systems.

We have been able to synthesise and characterize vanadium and rhenium complexes with the neutral hydrotris(1-pyrazolyl)methane $\text{HC}(\text{pz})_3$ (pz = pyrazolyl), e.g., $[\text{VCl}_3\{\text{HC}(\text{pz})_3\}]$ or $[\text{ReCl}_3\{\text{HC}(\text{pz})_3\}]$ or with the anionic analogue tris(1-pyrazolyl)methanesulfonate $[\text{SO}_3\text{C}(\text{pz})_3]$, namely $[\text{VCl}_3\{\text{SO}_3\text{C}(\text{pz})_3\}]$, $[\text{VOCl}\{\text{SO}_3\text{C}(\text{pz})_3\}\text{DMF}]$ or $[\text{ReOCl}_2\{\text{SO}_3\text{C}(\text{pz})_3\}(\text{PPh}_3)]$, and we have found⁴ that these complexes catalyse the peroxidative oxidation of cycloalkanes to the corresponding ketones and alcohols.

However, their syntheses often require an inconvenient reflux of dangerous solvents during several hours or days, what has encouraged us to use the microwave reactor.

We now report a fast, convenient and efficient synthetic method, assisted by microwave radiation, for the preparation of the above scorpionate vanadium and rhenium complexes. The effects of reaction conditions (e.g., temperature, pressure or type of solvent) are also indicated.

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7ª Conferência de
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Fátima, Portugal,
Dezembro de 2007.*

RHENIUM COMPLEXES AS CATALYSTS FOR THE BAEYER-VILLIGER OXIDATION

Lopes, Gonçalo¹; Alegria, Elisabete C.B.^{1,2}; Martins, Luísa M.D.R.S.^{1,2}; Pombeiro, Armando J.L.²

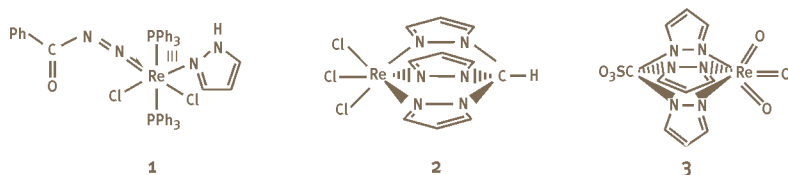
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² Centro de Química Estrutural, IST, Lisboa, Portugal

In spite of the expanded coordination chemistry for rhenium, the use of rhenium complexes as catalysts is still an underdeveloped field of research. However, the wide application of [(Me)ReO₃] (MTO) in oxidation catalysis clearly demonstrates the ability of this metal to form highly active catalysts for oxidation reactions of olefins and other unsaturated substrates. Hence, a contribution towards widening the use of Re complexes in catalysis is an objective of this work.

Recently we have found that some rhenium complexes with “scorpionate” nitrogen donor ligands, in particular the N₃ tripodal neutral hydrotris(1-pyrazolyl)methane (HC(pz)₃, Tpm) and the water soluble C-substituted sulfonate derivative tris(pyrazolyl)methanesulfonate (SO₃C(pz)₃, Tpm_s), can catalyse, in homogeneous systems, alkane functionalization reactions under mild or moderate conditions.

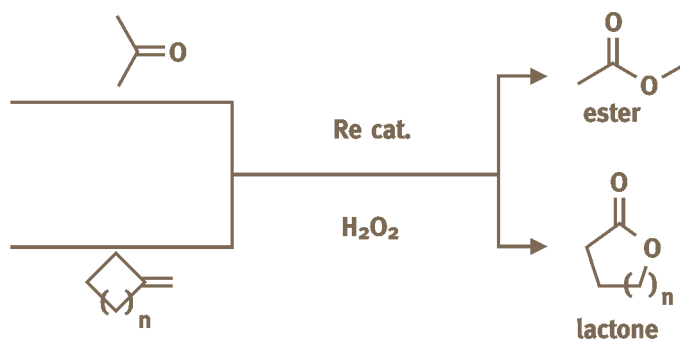
In pursuit of our interest on the catalytic activity of rhenium compounds we now report that the complexes [ReCl₂{N₂C(O)Ph}(Hpz)(PPh₃)₂] **1** (Hpz = pyrazole), [ReCl₃(HCpz₃)] **2** or [ReO₃(SO₃Cpz₃)] **3**, as



well as their precursors, [ReCl₂{η²-N,O-N₂C(O)Ph}(PPh₃)₂] and [ReOCl₂(PPh₃)₂], can act as catalysts (or catalyst precursors) for the Baeyer-Villiger oxidation of cyclic and acyclic ketones to the corresponding lactones or esters, by an aqueous diluted solution of H₂O₂, a green oxidant, under mild conditions:

Publicado em:

Livro de Abstracts do CIAM WORKSHOP, Laboratoire de Chimie de Coordination du CNRS, Toulouse, France, Dezembro de 2007.



The effects of a variety of factors, such as the type of catalyst, solvent, reaction time or temperature, were studied towards the optimization of the processes.

TREATMENT OF CORK PROCESSING WASTEWATERS BY ULTRAFILTRATION AND ULTRAFILTRATION INTEGRATED PROCESSES

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This work addresses the evaluation of membrane fouling in the ultrafiltration of cork processing wastewaters, rich in phenolic/tannic matter. To minimize UF fouling flocculation/flotation and ozonation pre-treatments were investigated.

The UF experiments were carried out in flat-sheet cells at transmembrane pressures of 1-3bar. A commercial membrane (Ropur-TS60) and four cellulose acetate laboratory-made membranes were used and their hydraulic permeabilities ranged from 7 to 110kg/h/m²/bar and the Molecular Weight Cut-Offs, MWCO, ranged from 4.5 to 86kDa.

The parameters studied were the permeate flux, rejection to organic matter, and rejection to phenolic/tannic compounds (gallic, protocatechuic, vanillic, syringic, ferulic and ellagic acids) and their identification and quantification was carried out through the use of HPLC. The compounds hydrophilicity/hydrophobicity was correlated to their rejection coefficients. The more hydrophobic component - ellagic acid - is almost totally retained and that independently of the membrane MWCO, transmembrane pressure, and feed flowrate leading to the conclusion of formation of an adsorption layer responsible for membrane fouling.

A flocculation study was carried out with chitosan and a Dissolved-Air-Flotation study was performed with the wastewater clarified by flocculation. The parameters varied were the operating pressure and the recycle-ratio. It was observed that for higher pressures and at a recycle-ratio of 0.19 the polyphenols removal was maximal. The flocculation/flotation pre-treatment led to the enhancement of the UF permeate fluxes reaching the 130%.

The ozonation pre-treatment was conducted in a batch reactor. The ozone-oxygen gas stream was fed to the reactor at a constant flowrate of 25l/h (at 1atm and 20°C). This pre-treatment lasted only 15min. and its objective was to oxidize selectively phenolic compounds. The ozone pre-treatment led to a reduction of 11% in the TOC content and to a reduction of 51% in the total polyphenols content, these reductions led to the enhancement of the UF permeate fluxes.

Publicado em:

Livros de Resumos da "Water Treatment and Re-Use Conference II", Tomar, Portugal, 11-16 de Fevereiro de 2007.

DEVELOPMENT OF NANOFILTRATION/STEAM STRIPPING SEQUENCE FOR COKE PLANT WASTEWATER TREATMENT

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The present work proposes the optimisation of an integrated process that consists in the coupling of Nanofiltration (NF) with Steam Stripping for the treatment of ammoniacal wastewaters contaminated by cyanides ions and phenols. These wastewaters are fractionated by NF into an ammonium concentrate and an ion-containing permeate stream. The concentrates are further fractionated in the steam stripping column.

The NF experiments were performed with a DSS plate and frame Lab-Unit 20, equipped with a HR-98-PP membrane. The NF experiments were run in concentration mode to optimise the concentrate ammonium content/permeate flux as a function of water recovery ratio (RR).

The optimisation of the NF/steam stripping integrated process was carried out with a sequential process simulator. The optimisation study showed that the NF should work at a recovery ratio of 40%. At this RR the ammonium can be efficiently concentrated and purified from cyanides at reasonable permeate flow rates. The column steam consumption was also optimised as a function of the NF concentrates flowrate. The integrated process leads to an increase of the stripping efficiency and to significant energy savings.

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Livros de Resumos do VI Congresso Ibero-Americano em Ciências e Tecnologias de Membranas, Campina Grande, Brasil, 8-11 de Julho de 2007.

ULTRAFILTRATION/NANOFILTRATION FOR SACCHARIDE FRACTIONATION

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The fractionation of saccharides and oligosaccharides by ultrafiltration(UF)/nanofiltration(NF) depends on: membrane pore size distribution, solutes concentration and pH. This work investigates the dependence of the fractionation of low molecular weight model-saccharide mixtures on the membrane molecular weight cut-off (MWCO) and on the solute concentration. The model saccharides tested were glucose, sucrose, lactose, raffinose and melezitose. Six laboratory made membranes were prepared according to the phase inversion method and five were further subjected to an annealing treatment. The membranes were characterised in terms of hydraulic permeability (L_p), MWCO and salts rejection (f). The UF/NF experiments with saccharide mixtures were performed in total recirculation mode and permeate samples are collected after the stabilization time. Feed recirculation flow rate is 33.5L/h. The saccharide fractionation is greatly influenced by the MWCO and by the feed solution composition. The increase of the total saccharide concentration led to an increase of the saccharide fractionation.

Publicado em:

Livros de Resumos do VI Congresso Íbero-Americano em Ciências e Tecnologias de Membranas, Campina Grande, Brasil, 8 - 11 de Julho de 2007.

A XAFS STUDY AT CERIUM K-EDGE IN COMPOUNDS FIGURING OUT VARIOUS CE-SPECIATIONS AND COORDINATION ENVIRONMENTS

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- 4 IST, Chem. Eng. Dept. Lisboa, & Univ. Aveiro, Dept. Ceramic and Glass Eng., Aveiro, Portugal

Publicado em:
*Livro de resumos
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 Conference of SPM
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 de Materiais) – IV
 International Materials
 Symposium – A
 Materials Science
 Forum, April, 1-4,
 Faculdade de
 Engenharia da
 Universidade do Porto,
 Porto, Portugal.*

The application fields of cerium compounds have enlarged in the last years. Cerium oxide is emerging as a hydrocarbon catalyst in self cleaning ovens and is now extensively used as a promoter in three-way catalysts (TWCs) for automotive emission control. This oxide allows for selective absorption of ultraviolet light in glass and, owing to its nonstoichiometric behaviour once the oxidation state of Ce can be 3^+ or 4^+ , CeO_2 also proved to be a good promoter for oxygen storage. The cerium oxide is also used in diesel fuels for a more complete combustion to abate soot formation. Moreover the magneto-optical signals of Ce-compounds have an outstanding figure of merit amongst other classes of magnetic materials.

Synchrotron radiation is nowadays a powerful means of studying X-ray absorption fine-structure spectroscopy (XAFS), either close to the absorption edge (XANES) or up to a hundred electron volts above the edge (EXAFS). The latter has revealed itself as an outstanding technique for structural characterization of catalytic systems.

As a preparatory approach to the characterization of corrosion behavior of bis-silane Ce-treated films over aluminum alloys, a XAFS study at the Ce K-edge in compounds with well-known crystal structure and chemical composition was undertaken at the ESRF[#] using the instrumental set-up of beamline BM29. The following prototypes were selected to model cerium speciations (valence plus coordination environment): synthetic CeO_2 (a cubic oxide with fluorite-type crystal structure and regular cubic coordination of Ce^{4+}), monazite (La-rich natural $CePO_4$ with a less regular environment of Ce^{3+} ions), octahydrated Ce^{4+} sulphate $Ce(SO_4)_2 \cdot 8H_2O$, and the hexa-hydrated Ce^{3+} nitrate $Ce(NO_3)_3 \cdot 6H_2O$. A discussion is presented on the local structure parameters extracted from collected EXAFS spectra, along with prospective comments concerning the role of cerium in the pre-treatment of bis-silane films deposited onto alloy substrates.

INFLUENCE OF INTERMETALLIC INCLUSIONS ON THE MANNESMANN EFFECT IN THE CROSS WEDGE ROLLING OF ENGINEERING STEELS

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The Cross Wedge Rolling (CWR) is a partial compression forming method where two wedge shaped tools are in counterrotating contact with the part and create rotation symmetric work-pieces (e.g.: axles, shafts, gearboxes) as well as preforms with optimum mass distribution for subsequent die forming (e.g.: levers, cranks, connecting rods, etc.). The CWR process offers some unique features like high form, mass precision of the work-pieces, higher output compared to machining methods, better material usage and very high quality performance. However, the internal voids that occur due to the Mannesmann effect in the axis of the forged parts appear as a major constraint to the development of this technology since it can lead to the catastrophic failure of products. Using an extensive metallurgical research, this work has studied the influence of intermetallic inclusions on the susceptibility of engineering steels to axial crack generation during CWR. Based on the experimental analysis of samples coming from interrupted and finished CWR tests, the origin of inner defects was investigated as a function of the material grade (20MnCr5, 16MnCr5, 30MSV6 and C70S6) and inclusions distribution. It was concluded that the MnS precipitates appear to have a prime role in the development of the Mannesmann effect.

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de Materiais) – IV
International Materials
Symposium – A
Materials Science
Forum, April, 1-4,
Faculdade de
Engenharia da
Universidade do Porto,
Porto, Portugal.*

CORROSION EVALUATION OF NANOPARTICLES CONTAINING POLYANILINE FILMS ON AL₃₁₀₅ ALLOY

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Conducting polymers like polyaniline, polypyrrole and their derivatives have been studied as corrosion protection coatings for aluminium and steel alloys. Recently, inorganic fillers, such as clays or metal oxides have been incorporated to improve the corrosion protection performance of conducting polymers.

The present work aims the evaluation of the corrosion protection of polyaniline films incorporating TiO₂ nanoparticles on 3105 aluminium alloy. The films have been deposited on aluminium by electro polymerisation of aniline in presence of the nanoparticles.

Electrochemical Impedance Spectroscopy (EIS) and Salt Spray Testing (SST) were used to evaluate corrosion resistance of the film. Scanning Electron Microscopy (SEM) was used to characterize the morphology of the coatings.

It was found that TiO₂ containing films had provided better corrosion protection of the 3105 aluminium alloy, both in EIS analysis carried out in NaCl solutions and in SST.

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*Livro de resumos X
IBERIC Meeting of
Electrochemistry/XIV
Encontro da
Sociedade Portuguesa
de Electroquímica,
12 – 14 Abril 2007,
Departamento de
Química, Faculdade de
Ciências e Tecnologia,
Universidade de
Coimbra, Coimbra,
Portugal.*

CORROSION PERFORMANCE OF NANOPARTICLE-CONTAINING POLYANILINE FILMS ON AA3105 ALUMINIUM ALLOY

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The chromates are highly effective as corrosion inhibitors as they show the self-healing property that it is difficult to emulate by other materials. The study of intrinsically conducting polymers as chromate replacement for corrosion protection is an active research area and several authors consider these polymers as electroactive corrosion inhibitors with potential self-healing properties. Conducting polymers, for example polyaniline, polypyrrole and their derivatives, have been studied as corrosion protection coatings for aluminium alloys and steel. Recently, inorganic fillers, comprising clays or metal oxides, have been incorporated to improve the corrosion protection performance of conducting polymers.

This work aims the evaluation of the corrosion protection performance of polyaniline coatings with TiO₂ nanoparticles on AA3105 aluminium alloy, obtained by aniline electropolymerisation and nanoparticle electrodeposition on the aluminium substrate.

Publicado em:

*Livro de abstracts
EUROCORR 2007,
The European
Corrosion Congress:
Progress by Corrosion
Control,
9-13 Setembro, 2007,
Freiburg im Breisgau,
Germany.*

NEW ORGANIC LIGANDS FOR ONLINEAR OPTICAL COMPLEXES

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Publicado em:
Livros de Resumos do
7th Portuguese
National Meeting of
Organic Chemistry,
1st Luso-French
Symposium, Lisboa,
16 a 18 de Julho de
2007.

The search for organometallic compounds with nonlinear optical (NLO) properties has becoming a field of considerable interest due to their potential as materials with technological applications in the area of nonlinear optical phenomena. In the organometallic push-pull systems, the metal center behaves as an electron-acceptor or electron-donating center bonded to an organic delocalized π -electron system. Organic compounds could present themselves NLO properties due to the high electronic polarizability of their π -system. The ability to introduce subtle changes in the chemical structures leading to important improvements in their properties and to build structure-property relationships, make the organic compounds still good candidates for electronics and optical phenomena investigation area.

Here, we present the synthesis and spectroscopic characterization of electron-withdrawing organic ligands, suitable for coordination to electron donating Fe or Ru metal centers. These ligands present a two aromatic rings backbone linked by a spacer (double, triple or hydrazone bond) with one or two electron withdrawing nitro groups on *para* and *ortho* positions of the second aryl ring (Figure 1). The substitution with a nitrile or alkyne groups provide an available site for coordination to the metals. The structures of several compounds were confirmed by X-Ray diffraction studies.

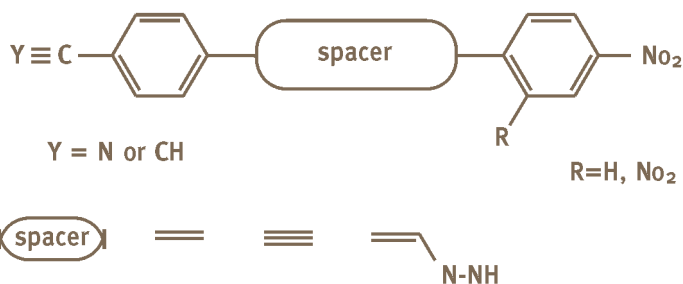


Figure 1.

SYNTHESIS OF IRON(II) AND RUTHENIUM(II) NITRILE AND ACETYLIDE COMPLEXES: NEW BUILDING BLOCKS FOR MOLECULAR WIRES?

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Molecular wires comprising mixed-valence bimetallic units or remote redox-active organometallic groups linked by conjugated bridging organic chains could be exploited in molecular electronics and opto-electronic devices.

The metallomolecular wires are constituted by an organic spacer (molecular bridge) and a metal centre, being both parts responsible for the final performance of the molecular wire. The organic spacers are responsible for the length and electronic properties and the metal centres introduce electrons in the system, increasing conductivity.

Nitrile and/or alkynyl ligands can offer synthetic and structural versatility and the metal nitrile and acetylide linkages has proven to be useful to obtain rich complexes with an extended π -conjugation. Their contribution is also essential for the building of molecular wires constituted of bimetallic complexes, allowing electronic communication between redox-active terminal end groups through delocalized bonds.

Publicado em:

Livros de Resumos do VII^a Conferência de Química Inorgânica da Sociedade Portuguesa de Química, Fátima, 30 Novembro e 1 de Dezembro de 2007.



We report in this communication, the synthesis of several iron(II) and ruthenium(II) nitrile and/or acetylide complexes based on different organic spacers, such as NC-CH₂-CN, NC-C₆H₄-CN and NC-C₆H₄-CCH, and different metallic fragments ([CpFe(dppe)]⁺, [CpFe(CO)₂]⁺, [CpRu(dppe)]⁺, etc. For the complexes obtained, UV-Vis, IR and NMR spectroscopies and electrochemical studies by cyclic voltammetry will be used to evaluate the efficiency of the electronic interaction between the metal centres along the bridging systems.

NOVEL IRON(II) COMPLEXES WITH OLIGOPYRIDINE LIGANDS: SYNTHESIS, CHARACTERISATION AND ELECTROCHEMICAL STUDIES

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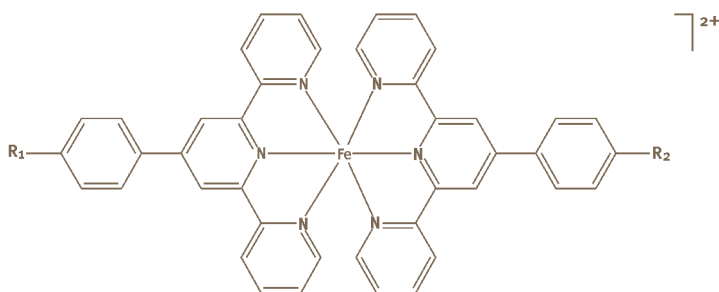
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Publicado em:
 Livros de Resumos do
 VII^a Conferência de
 Química Inorgânica da
 Sociedade Portuguesa
 de Química, Fátima,
 30 Novembro e 1 de
 Dezembro de 2007.

The exploitation of organometallic and coordination compounds as new materials with nonlinear optical (NLO) properties, motivated by their potential technological applications, has been during the past decades, a growing area of research. The introduction of helically shaped systems, allows measurable dipolar and magnetic contributions to NLO effects, which is an area of interest for photorefractive materials.

Oligopyridines and ligands incorporating multiple oligopyridine metal-binding domains have proved to be ideal touchstones for probing metal-directed helicate assembly processes. Metal complexes with oligopyridines, such as terpyridines, although extensively studied for their photochemical and photophysical properties, have not been explored as potential NLO materials.

We report herein the synthesis of terpyridine derivatives and their coordination to iron(II) fragments, such as $[\text{CpFe}(\text{dppe})]^+$ (figure 1). The new complexes were characterised by the usual spectroscopic UV-Vis, IR and NMR techniques and their electrochemical behaviour explored by cyclic voltammetry.



$R_1 = \text{H}, \text{CN}, \text{N}(\text{CH}_3)_2, [\text{CpFe}(\text{dppe})\text{NC}]$, $R_2 = \text{N}(\text{CH}_3)_2, \text{NO}_2, \text{CN}, [\text{CpFe}(\text{dppe})\text{NC}]$

Figure 1. Terpyridine derivatives.

NOVEL IRON(II) AND RUTHENIUM(II) COMPLEXES WITH OLIGOPYRIDINES LIGANDS IN HELICAL ENVIRONMENTS

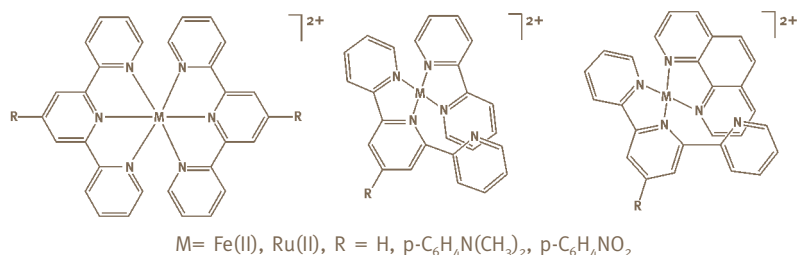
Jacob, C.I.¹; Robalo, M.P.^{1,2}; Garcia, M.H.³;
Piedade, M.F.M.^{1,3}; Duarte, M.T.¹; Dias, A.R.¹

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The exploitation of organometallic and coordination chemistry for the synthesis of new compounds with nonlinear optical (NLO) properties, motivated by their potential technological applications in telecommunication and computer industries, has been during the past decade, a growing area of research.

The introduction of helically shaped systems, allows the presence of measurable dipolar and magnetic contributions to NLO effects, which is an area of interest for photorefractive materials. Magnetic contributions to NLO effects, though small, can be important in new generations of devices which will allow easier fabrication as centrosymmetric structures will then be acceptable.

Oligopyridines and ligands incorporating multiple oligopyridine metal-binding domains have proved to be ideal touchstones for probing metal-directed helicate assembly processes. Metal complexes of oligopyridines, such as terpyridines, have been extensively studied for their photochemical and photophysical properties, however from a NLO point of view those metal complexes have been few investigated. We report herein the synthesis and characterisation of terpyridine derivatives and the coordination of these ligands to iron(II) and ruthenium(II).



The new complexes were characterised by the usual spectroscopic UV-Vis, IR and NMR techniques and for some intermediates X-ray diffraction studies were also performed.

Publicado em:

*Livros de Resumos do
XVIth FECEM
Conference on
Organometallic
Chemistry, Sofia,
1 a 6 de Setembro de
2007.*

THIOXANTHONES AND THIOXANTHIONES: PROMISING ORGANIC NLO MATERIALS?

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Piedade, M.F.M.^{1,3}; Duarte, M.T.¹; Goovaerts, E.⁴;
Wenseleers, W.⁴; Campo, J.⁴

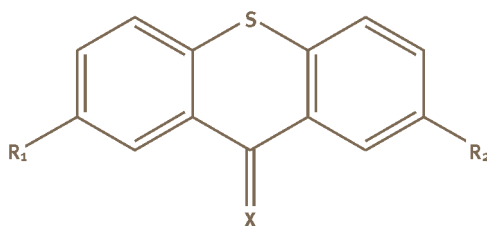
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The search for new organic molecules or metal transition coordination complexes with high values of hyperpolarizability β has been an area of interest during the last twenty years, due to their potential technological applications in telecommunication and computer industries.

Current NLO devices generally rely on inorganic crystals, but such materials can be expensive, fragile and difficult to integrate into devices. Organic materials offer several advantages, such as large non-linear coefficients, high optical damage thresholds, ease of processing and the possibility of tailoring compounds to the precise requirements of the device.

Publicado em:

*Livros de Resumos do
Primer Simposio
Iberamericano de
Química Orgánica
(SIBEAQO I), Mar del
Prata, 11 a 16 de
Novembro de 2007.*



$R_1 = \text{NH}_2, \text{CCH}, \text{CN}, \text{NO}_2$
 $R_2 = \text{NO}_2$
 $X = \text{O}, \text{S}$

We report herein the synthesis and characterisation of several thioxanthones and thioxanthiones units. These new organic molecules were characterised by the usual spectroscopic IR, ^1H and ^{13}C NMR techniques. Measurements of the molecular quadratic hyperpolarizabilities of these molecules were carried out by HRS at the fundamental wavelength of 1550 nm in liquid solution. The high experimental β values were correlated with spectroscopic data and with X-ray diffraction studies in order to understand the molecular structure-NLO property relationship.

AVALIAÇÃO DO POTENCIAL ANTIOXIDANTE DO MEL DA REGIÃO DA LOUSÃ

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Nos últimos anos tem-se assistido a uma intensa pesquisa sobre as propriedades antioxidantes de produtos naturais. O conhecimento das importantes funções que os antioxidantes desempenham na inibição dos radicais livres resultantes do metabolismo celular, tem motivado o interesse pela análise destes compostos em diversos produtos alimentares.

No âmbito do projecto de investigação aplicada Avaliação do Potencial Antioxidante do Mel Nacional, desenvolvido em colaboração com a Lousãmel e financiado pelo Ministério da Agricultura, das Pescas e do Desenvolvimento Rural, foram recolhidas amostras de mel da colheita de 2005 provenientes das regiões da Lousã, Góis e Figueiró dos Vinhos. A caracterização da actividade antioxidante foi efectuada através da determinação dos teores em compostos fenólicos e flavonóides, da quantificação dos antioxidantes e da avaliação da capacidade de aprisionamento de radicais livres, usando métodos de espectrometria de absorção molecular na zona do visível.

Em simultâneo foi realizado um estudo semelhante com méis designados como monoflorais, provenientes de quatro regiões distintas de Portugal, com o objectivo de estabelecer comparações e de modo a tentar encontrar eventuais relações entre a origem floral e a capacidade antioxidante. Nesse sentido foram analisados os méis de trevo e incenso dos Açores, eucalipto da Beira Litoral, laranja do Algarve e urze da Beira Baixa.

Os resultados mostraram que o teor em compostos fenólicos variou significativamente com o tipo de mel analisado. Os méis da Lousãmel apresentaram uma elevada concentração em polifenóis, mas inferior à determinada no mel de urze. Dos méis analisados, o mel de laranja foi o que apresentou uma menor concentração nestes compostos.

Em relação aos flavonóides, foram encontrados nos méis da Lousãmel e nos de trevo, incenso e urze teores muito semelhantes e consideravelmente superiores aos apresentados pelo mel de eucalipto.

O mel de urze apresentou um teor em compostos antioxidantes consideravelmente superior ao encontrado nos outros méis. Os méis da Lousãmel revelaram, também, um teor significativo nestes compostos.

Publicado em:

*Documentação do 8º
Fórum de Apicultura,
Boticas, 17 de
Novembro de 2007.*

Os teores mais baixos foram encontrados nos méis de laranja e incenso.

Quanto à capacidade de resgate de radicais livres de 2,2 difenil-1-picrilhidrazil, expressa através do parâmetro IC_{50} , os méis da Lousã-mel e o mel de urze foram os que mostraram maior capacidade de inibição dos radicais ao contrário do mel de laranja que revelou ser o menos eficaz.

Ao relacionar todos os parâmetros em estudo encontrou-se uma boa correlação entre o teor em compostos fenólicos, a cor e as características antioxidantes.

ACTIVIDADE ANTIOXIDANTE DE PRODUTOS HORTÍCOLAS

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Os antioxidantes desempenham funções de reconhecida importância na manutenção da saúde e na prevenção de doenças associadas ao envelhecimento. As propriedades antioxidantes destes compostos contribuem, também, para a manutenção da qualidade de produtos alimentares, uma vez que são responsáveis por retardar processos de degradação em alimentos.

Os estudos desenvolvidos nos últimos anos têm permitido conhecer a actividade antioxidante de uma grande diversidade de produtos naturais e apresentam um papel relevante no desenvolvimento de alimentos funcionais e na procura de conservantes para aplicação na indústria alimentar.

Através da avaliação da actividade antioxidante de produtos hortícolas de cultivo frequente em Portugal, pretende-se obter informações que possam contribuir para a valorização junto do consumidor de alguns destes produtos por se tratarem de uma possível fonte de antioxidantes.

O presente trabalho envolve um estudo comparativo da actividade antioxidante da couve-galega, nabiça e acelga. Os extractos destes vegetais foram preparados a partir de técnicas de extracção com solventes e recorrendo a uma sonda de ultrassons, no sentido de promover uma maior eficiência na extracção.

A quantificação dos compostos fenólicos nos diversos extractos foi realizada através de espectroscopia de absorção molecular no visível, segundo o método de Folin-Ciocalteu e utilizando uma curva de calibração com ácido gálico. A actividade antioxidante dos extractos foi determinada avaliando a sua acção inibidora sobre radicais de 2,2-difenil-1-picrilhidrazil (DPPH) através de medidas de absorvância a 517nm e recorrendo a uma curva de calibração com ácido ascórbico.

Os resultados indicaram para os extractos de couve-galega e nabiça um maior teor em compostos fenólicos assim como uma actividade antioxidante mais elevada. Apesar dos extractos de acelga apresentarem uma menor acção antioxidante, os vegetais em estudo neste trabalho podem, de um modo geral, constituir fontes dietéticas de antioxidantes sendo de estimular o seu consumo junto da população.

Publicado em:

Livros de Resumos do 6º Encontro da Divisão de Química Analítica, "SPQ-Analítica'07", IST, Lisboa, 29 e 30 de Março de 2007.

POLIFENÓIS EM VEGETAIS DE USO TRADICIONAL NA COZINHA PORTUGUESA

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Publicado em:
*Livro de Resumos do
8º Encontro de
Química dos Alimentos
– Alimentos
Tradicionais, Alimentos
Saudáveis,
Rastreabilidade, Escola
Superior Agrária de
Beja, Beja, 4 – 7 de
Março de 2007.*

A quantificação dos compostos fenólicos em extractos de couve galega, nabiça, acelga e rucola foi realizada por espectroscopia de absorção molecular no visível, segundo o método de Folin-Ciocalteu e recorrendo a uma curva de calibração com ácido gálico. A extração dos polifenóis da matriz vegetal, fresca ou seca e previamente homogeneizada, foi realizada com etanol à temperatura ambiente e auxiliada através da aplicação de ultrassons. O teor em compostos fenólicos nos extractos das plantas frescas variou entre 16,8 e 8,8mgAG/g matéria seca, apresentando os extractos de couve galega e nabiça a concentração mais elevada e com valor semelhante. Nos extractos de rucola observou-se o menor teor em polifenóis enquanto que nos de acelga se determinou uma concentração média de $13,0 \pm 1,4$ mgAG/g matéria seca. A determinação dos compostos fenólicos nos extractos das amostras previamente sujeitas ao processo de secagem, conduziu a valores inferiores cerca de 70 a 80% aos determinados a partir das plantas frescas, com a excepção da rucola em que se observou uma redução de aproximadamente 45%.

DERIVING AN INDOOR ENVIRONMENTAL INDEX FOR PORTUGUESE OFFICE BUILDINGS

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Departamento de Engenharia Química, ISEL, Lisboa, Portugal

The EC issued a Directive in 2002 aiming to reduce the energy consumption of buildings, which was adopted by the EU member states and came into force in 2006. Portugal adopted it by issuing law decrees in 2006 which considered not only the energy saving aspects but also additional specific measures aiming to protect indoor air quality (IAQ). This new legislation is now being enforced and it will be necessary to define compliance acceptance levels for the prescribed indoor air limits. The use of comfort or environmental indexes could be of considerable help in order to ameliorate the evaluation of indoor air quality. This paper presents a proposal of an index regarding IAQ which is an index considering both the aspects of thermal comfort and toxicity. The use of this index is now being evaluated using observed concentrations in real office environments.

Publicado em:

*Proceedings SBo7-
Sustainable
Construction Materials
and Practices, Lisboa,
2007.*

REFLEXIONS ON THE USE OF RENEWABLE POWER SOURCES AND NUCLEAR ENERGY IN PORTUGAL

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Publicado em:
*Proceedings 4th
European Congress on
Economics and
Management of Energy
in Industry, Porto,
2007.*

This paper analyses the current energy balance of Portugal, considering the actual sources which are mainly traditional fossil fuels, hydraulic power and renewables. Also, other potential sources are discussed and taken into consideration in view of the previewed evolution of the country in energetic terms. Among these, nuclear power, which was once regarded as an option, but its implementation was delayed, is now being considered again. This paper also sums up the main issues to be considered in a future debate on the subject.

HOW TO MEASURE CUSTOMER SATISFACTION IN VIEW OF THE QUALITATIVE JUDGMENTS OF THE CUSTOMER?

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A new method for measuring and analyzing customer satisfaction is presented. The mathematical model expresses the fundamental relationship between criteria and the overall utility which expresses the global customer satisfaction. The procedure used to estimate the basic model is dummy variable regression with constraints. The method can very simply consider nonmetric data by codification of the criteria levels so in that way is possible to consider the qualitative judgments and preferences of the customer. The method accounts for the non-linear response of customer satisfaction to the performance of different product/service criteria. The main advantages of the method are discussed and future research about this topic is proposed.

Publicado em:

*Proceedings das XIV
Jornadas de
Classificação e Análise
de Dados, Porto,
8-12 Fevereiro de
2007, pp.95-100 (ISBN
978-972-8688-50-9).*

AN ALTERNATIVE TO THE MUSA METHOD FOR CUSTOMER SATISFACTION ANALYSIS

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This paper presents an alternative to the MUSA method. The aggregation of the individual customer satisfaction criteria into an overall value function uses dummy variable regression with constraints employing the least squares approach. The value of each level of the piecewise value function is calculated considering that the coefficient of each dummy variable represents the difference of value of that level to a reference level. The plot of the value functions and the relative weights provide a basis for a straightforward interpretation of the results.

Publicado em:

*Proceedings do 22nd
European Conference
on Operational
Research, Praga,
8-1 de Julho de 2007
pp. 120.*

DESIGN OF EXPERIMENTS IN CHEMICAL ENGINEERING EDUCATION. APPLICATION TO LIQUID-LIQUID EXTRACTION

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The introduction of experimental design methodology at the earliest stage of the development cycle, where new products are designed, existing products designs improved and manufacturing processes optimized, is often the key to overall product success (Montgomery, 2005). Improving the quality of products and processes with reduced costs represents an economical and technological challenge for engineers. Experimental design methods are very useful to reach these goals. Designed experiments can be used in chemical engineering laboratory work to improve the learning of these kind of statistical tools enhancing the future utilization by the chemical engineering graduates. It is presented two case studies concerning the utilization of a liquid-liquid extraction equipment used for educational purposes. The first case study concerns the operation of the equipment in a continuous operation mode and a second case study concerning the batch mode. In both operation modes it is required that the students identify which variables are most influential on the response and also determine the regression model that fits the data.

Publicado em:

ISI 2007 Book of abstracts 56th Session of the International Statistical Institute, Lisboa, Portugal, 22-29 August 2007, pp. 657-658. Bulletin of the International Statistical Institute 56th Session Proceedings in CD.

BIOCATALYSIS OF *Coriolus versicolor* BIOMASS CONTAINING GLUCOSE 2-OXIDASE ACTIVITY AT HIGH PRESSURES

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Publicado em:
*Proceedings of 5th
International
Symposium on High
Pressure Processes
Technology and
Chemical Engineering,
Segovia, 24 to 27 of
June of 2007, pp. 1-4.*

The present work involves the conversion of D-glucose into D-glucosone in the presence of *Coriolus versicolor* biomass at high pressures with compressed air in a modified commercial reactor. Several parameters affecting biocatalysis at high pressures, up to 20MPa, were investigated as follows: temperature, pressure, pH, biomass concentration and glucose concentration. The data presented in this work strongly suggests that the rate of reaction increases with temperature, pressure and glucose concentration. The optimum temperature and pH for conversion of D-glucose into D-glucosone was 55°C and at pH 5.0, respectively.

On the other hand, the kinetic constants (*i.e* Km and Vmax) were also determined at high pressure which was found to be 2.95mM and 8.8U/mg protein for Km and Vmax, respectively.

The use of biomass containing glucose 2-oxidase activity was also useful for conversion of D-glucose into D-glucosone. Moreover, the re-utilization of biomass for this conversion at high pressure revealed that the yield was about 50%.

SUPERCRITICAL FLUID EXTRACTION, HYDRODISTILLATION AND SOXHLET EXTRACTION OF THE AERIAL PART OF WINTER SAVORY: COMPARATIVE EVALUATION OF THE EXTRACTION METHOD ON THE CHEMICAL COMPOSITION

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Supercritical fluid extraction of the volatile oil of the aerial part of the winter savory was carried out in different conditions of pressure, temperature, mean particle size and CO₂ flow rate and the results were compared with those obtaining by hydrodistillation with a Clevenger-type apparatus. The non-volatile components were extracted by SFE at higher pressures and by soxhlet extraction with different solvent mixtures. Concerning the volatile components, although the extraction yields of SFE and HD are quite similar, SFE extracts are richer in thymoquinone, a component with interest to the pharmaceutical industry due to its anti-cancer, antioxidant and anti-inflammatory properties.

Publicado em:

Proceedings of European Congress of Chemical Engineering, Copenhagen, 16 e 20 of September of 2007, pp. 1-4.

DESIGN OF EXPERIMENTS IN CHEMICAL ENGINEERING EDUCATION. APPLICATION TO LIQUID-LIQUID EXTRACTION

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Publicado em:

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abstracts 56th Session
of the International
Statistical Institute,
Lisboa, Portugal,
22-29 August 2007,
pp. 657-658. Bulletin
of the International
Statistical Institute 56th
Session Proceedings
in CD.*

The introduction of experimental design methodology at the earliest stage of the development cycle, where new products are designed, existing products designs improved and manufacturing processes optimized, is often the key to overall product success. Improving the quality of products and processes with reduced costs represents an economical and technological challenge for engineers. Experimental design methods are very useful to reach these goals. Designed experiments can be used in chemical engineering laboratory work to improve the learning of these kind of statistical tools enhancing the future utilization by the chemical engineering graduates.

It is presented two case studies concerning the utilization of a liquid-liquid extraction equipment used for educational purposes. The first case study concerns the operation of the equipment in a continuous operation mode and a second case study concerning the batch mode. In both operation modes it is required that the students identify which variables are most influential on the response and also determine the regression model that fits the data.

ESPUMAS CERÂMICAS COMO SUPORTES CATALÍTICOS

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Espumas reticulares de cordierite desenvolvidas por um método de polimerização “*in situ*” revelaram propriedades de elevado interesse para a aplicação como suportes catalíticos. Estas espumas são caracterizadas por possuírem porosidades superiores (>90%) às obtidas pelo método de replicação polimérica (70-85%). O desenvolvimento de um método de revestimento de espumas cerâmicas com catalisadores zeolíticos, e a optimização de parâmetros como teor de sólidos, ligante, surfactante ou pré-revestimento da espuma, tem estado a ser efectuado. As melhores características foram observadas para espumas com aproximadamente 17% p/p) de revestimento obtidas a partir de suspensões com cerca de 16% de teor de sólidos. Espumas revestidas com zeólitos Pt/ZSM5 estão a ser utilizadas como catalisadores para a combustão catalítica de COVs, nomeadamente isopropanol e tolueno.

Publicado em:

Actas do 8º Encontro Nacional da Divisão de Catálise e Materiais Porosos da Sociedade Portuguesa de Química, Lamego, 21-23 Setembro 2007, pp. 45-48.

STRUCTURE OF CORDIERITE FOAMS PREPARED BY DIRECT FOAMING

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Open-cell ceramic foams are gaining increasing interest in a variety of technological applications that include filters for molten metals, diesel particulate traps, heat exchangers, thermal and electric insulators and catalyst supports. This is associated with their intrinsic properties, namely high permeability, high surface area, low conductivity, low mass and excellent resistance to chemical corrosion. Amongst the various materials that can be used, cordierite is known to combine relatively low thermal expansion needed for thermal shock resistance with relatively high refractoriness for operating in severe exhaust environments at high temperatures, which makes it suitable for catalyst supports.

In this work, we proposed a new direct foaming process to produce open-cell cordierite foams. The production method is based on a conventional polyurethane system made with two components, which consists in the addition of the ceramic particles to the polyol resin and to the isocyanate, then the mix of the two components give rise to the formation of the polyurethane/ceramic foam. Experimental parameters such as the type and amount of surfactant, catalyst, polyol as well as the content of solids, blowing agent and plasticizer were optimized. After curing, the polymer component of the PU/ceramic foam was burnt out in air, followed by sintering of the ceramic material. The resulting ceramic foams consisted of a highly interconnected network of cells with densities as low as 9% of theoretical. Densities in the range of 130-250kg m⁻³ were obtained. Both the green and the sintered ceramic foams structures were characterised by optical microscopy and scanning electron microscopy (SEM), revealing an open-cell structure very attractive for catalyst support purposes (Fig.1). Attempts have been made in order to control the pore structure since it directly affects the physical properties, namely the mechanical strength. In this respect, the use of a dip-coating method to improve the strength of the resulting foams has been discussed.

Publicado em:

*Actas do Materiais
2007, Porto 1-4 April
2007, pp.14.*

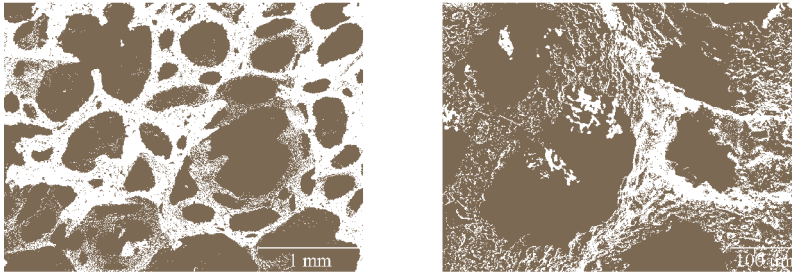


Figure 1. Sem micrograph showing the structure of a cordierite foam.

COUVES CHUMBADAS

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Publicado em:
*Actas do 8º Encontro
de Química dos
Alimentos, Beja, 4 a 7
de Março de 2007,
pp. 277-282.*

Actualmente é frequente constatar a existência de pequenas áreas de exploração agrícola (hortas) junto de vias de elevada intensidade de tráfego automóvel, onde uma variedade significativa de géneros alimentícios é cultivada. Estas pequenas “hortas” são geralmente exploradas por camadas da população com fracos recursos económicos, e aposentados que visam ocupar algum do seu tempo livre. Uma preocupação que emerge desta prática, prende-se com o consumo humano dos referidos alimentos. De facto, um número significativo de indivíduos consome produtos agrícolas provenientes destas zonas de cultivo, pensando estar a consumir alimentos saudáveis, livres de quaisquer agentes químicos, quando na realidade está a prejudicar significativamente a sua saúde. Se pensarmos que o tráfego automóvel é, nomeadamente em zonas de média e baixa actividade industrial, a principal fonte de agentes poluentes da atmosfera, com particular destaque para os metais tóxicos, passíveis de se depositarem nos solos adjacentes, então, obrigatoriamente, o problema deve ser encarado com uma maior seriedade. Este aspecto torna-se ainda mais preocupante quando algumas autarquias não só não limitam ou impedem a proliferação deste tipo actividade, como inclusivamente a fomentam, com a recuperação de alguns taludes situados em bermas de estradas. Neste trabalho apresentam-se os resultados de um estudo realizado em couves portuguesas que mostra, efectivamente, a presença de metais tóxicos, nomeadamente chumbo e cádmio, em amostras recolhidas numa zona de cultivo situada nas bermas do IC 19. A determinação dos metais foi efectuada por intermédio de uma técnica electroanalítica designada Voltametria de Redissolução Anódica de Onda Quadrada (SWASV), aplicada no caso presente a alimentos. Estes ensaios foram efectuados após digestão ácida por tecnologia de microondas visando a destruição dos componentes orgânicos e a extracção dos elementos metálicos. Neste trabalho foi também realizado um estudo das amostras de couve recolhidas a diferentes distâncias da via de circulação com o objectivo de estudar o perfil de deposição dos gases de escape dos veículos automóveis com a distância à fonte de emissão. Compararam-se, ainda, estes resultados

com os obtidos na análise de uma couve portuguesa não exposta a agentes poluentes. Por fim foram analisadas couves portuguesas adquiridas em várias superfícies comerciais na perspectiva de que, sendo géneros alimentícios prontamente disponíveis para os consumidores, não é, por estes, conhecida a sua origem e locais de cultivo. Desta forma pretendeu concluir-se se de facto estaremos a consumir couve portuguesa com um teor em metais tóxicos manifestamente inferior ao caso das couves plantadas junto de zonas de elevada intensidade de tráfego automóvel ou se simplesmente a diferença não é tão significativa quanto, à partida possamos pensar. A prevalência de metais tóxicos nos géneros alimentícios cultivados junto às vias de tráfego reforça a necessidade de uma vigilância permanente da qualidade alimentar. Será, também, de equacionar a implementação de legislação que defina claramente as condições e locais admissíveis para cultivo de géneros alimentícios.

DIGESTÃO ANAERÓBIA DE RESÍDUOS SÓLIDOS ORGÂNICOS – FRUTAS, VEGETAIS E RELVA

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do Ambiente, Aveiro,
18 a 20 de Abril de
2007, pp. 1011-1017.*

A digestão anaeróbia é uma das tecnologias mais correntemente utilizadas no tratamento de resíduos sólidos orgânicos (RSO), dado que associa o tratamento à valorização dos mesmos. Em Portugal são produzidas quantidades muito significativas de RSO e existe uma carência acentuada de aplicações de digestão anaeróbia, tornando pertinente estudar este processo de tratamento e os substratos a serem degradados. Neste estudo pretendeu avaliar-se a capacidade de digestão anaeróbia de substratos compostos por vegetais, frutas e relva, tendo sido ensaiados dois reactores (*batch*) de 10L, em condições mesófilas. A digestão do substrato contendo 50% de vegetais e frutas e 50% de relva conduziu a uma produção de 479 mLCH₄/g SV e a do substrato com 25% de vegetais e frutas e 75% de relva a 363 mLCH₄/g SV.

ANAEROBIC DIGESTION OF FRUITS, VEGETABLES AND GRASS A CONTRIBUTION TO THE STUDY OF THE BIODEGRADABLE FRACTION OF MUNICIPAL SOLID WASTES

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In order to evaluate the anaerobic digestion profile of mixtures of fruits, vegetables and grass, the present study was undertaken. Two different mixtures were used using the same inoculum/substrate (I/S) ratio, mixture 1, comprising 50% of fruits and vegetables and 50% of grass, presents a greater methane production than mixture 2 which contain 25% of fruits and vegetables and 75% of grass. For both mixtures, it was found that a greater methane production resulted when a I/S ratio of 1 was used, as compared to I/S ratio of 2. The maximum specific methane production (0.434 L/gSV) was achieved by mixture 1 with I/S of 1.

Publicado em:

Proceedings do XI International Waste Management and Landfill Symposium, Sardenha, Itália, 1 a 5 de Outubro de 2007.

ESTRATÉGIAS E TECNOLOGIAS MAIS ADEQUADAS PARA O TRATAMENTO DE RESÍDUOS SÓLIDOS, COM VALORIZAÇÃO ENERGÉTICA

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Publicado em:

Proceedings da Conferência Engenharias'07 – Inovação e Desenvolvimento, Covilhã, 21 a 23 de Novembro de 2007, pp. 873-881.

Neste artigo, pretende-se abordar as estratégias de gestão de resíduos sólidos, à luz da legislação nacional e comunitária nesta matéria, bem como as melhores tecnologias aplicadas às mais importantes fileiras de resíduos, nomeadamente, urbanos e industriais, perigosos e banais. As várias opções tecnológicas para o tratamento, por valorização ou por eliminação de resíduos, assenta em variadas vertentes, nomeadamente, de viabilidade técnica e funcional, legal, económica e, por último, mas não menos importante, ambiental. Um dos objectivos deste artigo, é comparar as várias tecnologias competitivas entre si, nomeadamente, através das mais-valias ambientais e energéticas obtidas. É possível concluir, por exemplo, que, face às imposições legais comunitárias em matéria de reciclagem de resíduos e de minimização da utilização de aterros, está aberta uma grande janela de oportunidade para o desenvolvimento dos métodos biológicos com valorização material/energética, como a Compostagem e a Digestão Anaeróbia, para tratamento dos resíduos de fracção orgânica biodegradável. Os métodos de incineração aplicam-se essencialmente aos resíduos perigosos e que não possam ser sujeitos a outras alternativas de tratamento.

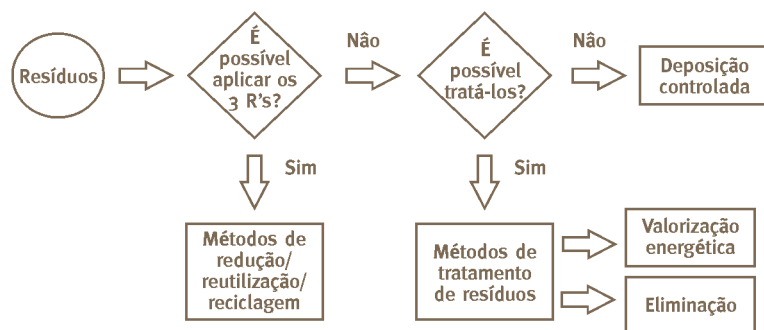


Figura 1. Metodologia hierárquica de gestão de resíduos sólidos.

Os métodos de tratamento actualmente existentes para tratar as várias fileiras de resíduos que não sejam passíveis de serem reutiliza-

dos ou reciclados, segundo o princípio de hierarquização de gestão de resíduos, subdividem-se da seguinte maneira, consoante o seu carácter de perigosidade: Tratamentos biológicos: Compostagem e Digestão Anaeróbia; Tratamentos térmicos com valorização energética: Incineração Dedicada, Co-Incinerção e Pirólise por Plasma com Vitri-ficação (PPV); Tratamentos físico-químicos.

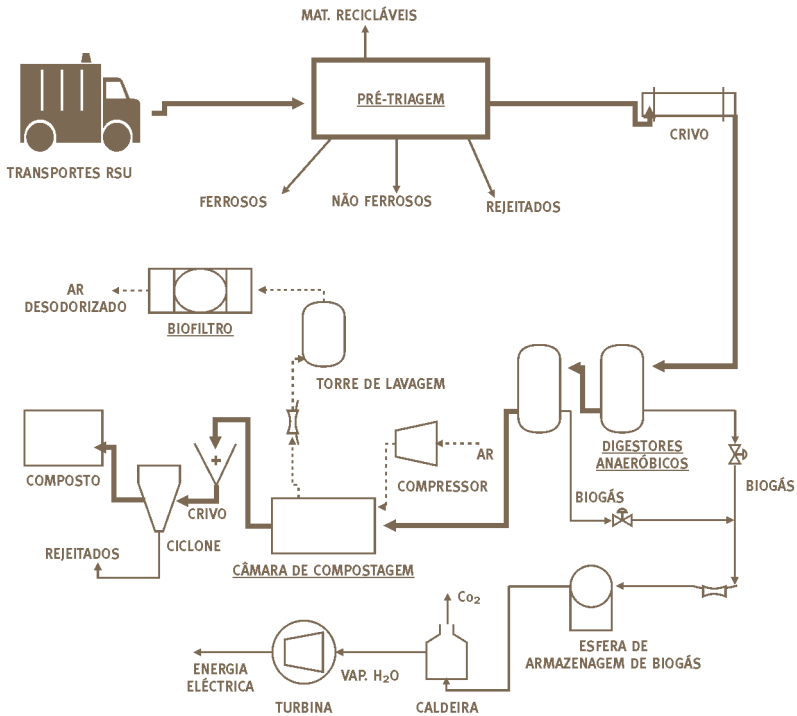


Figura 2. Flow-sheet genérico de um processo de Digestão Anaeróbia.

DEVELOPMENT OF NANOFILTRATION/STEAM STRIPPING SEQUENCE FOR COKE PLANT WASTEWATER TREATMENT

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Publicado em:
Proceedings do VI Congresso Íbero-Americano em Ciências e Tecnologia de Membrana, Campina Grande, Brasil, 8-11 de Julho de 2007, CD-ROM.

The present work proposes the optimisation of an integrated process that consists in the coupling of Nanofiltration (NF) with Steam Stripping for the treatment of ammoniacal wastewaters contaminated by cyanides ions and phenols. These wastewaters are fractionated by NF into an ammonium concentrate and an ion-containing permeate stream. The concentrates are further fractionated in the steam stripping column.

The NF experiments were performed with a DSS plate and frame Lab-Unit 20, equipped with a HR-98-PP membrane. The NF experiments were run in concentration mode to optimise the concentrate ammonium content/permeate flux as a function of water recovery ratio (RR).

The optimisation of the NF/steam stripping integrated process was carried out with a sequential process simulator. The optimisation study showed that the NF should work at a recovery ratio of 40%. At this RR the ammonium can be efficiently concentrated and purified from cyanides at reasonable permeate flow rates. The column steam consumption was also optimised as a function of the NF concentrates flowrate. The integrated process leads to an increase of the stripping efficiency and to significant energy savings.

ULTRAFILTRATION/NANOFILTRATION FOR SACCHARIDE FRACTIONATION

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The fractionation of saccharides and oligosaccharides by ultrafiltration(UF)/nanofiltration(NF) depends on: membrane pore size distribution, solutes concentration and pH. This work investigates the dependence of the fractionation of low molecular weight model-saccharide mixtures on the membrane molecular weight cut-off (MWCO) and on the solute concentration. The model saccharides tested were glucose, sucrose, lactose, raffinose and melezitose. Six laboratory made membranes were prepared according to the phase inversion method and five were further subjected to an annealing treatment. The membranes were characterised in terms of hydraulic permeability (L_p), MWCO and salts rejection (f). The UF/NF experiments with saccharide mixtures were performed in total recirculation mode and permeate samples are collected after the stabilization time. Feed recirculation flow rate is 33.5L/h. The saccharide fractionation is greatly influenced by the MWCO and by the feed solution composition. The increase of the total saccharide concentration led to an increase of the saccharide fractionation.

Publicado em:

Proceedings do VI Congresso Íbero-Americano em Ciências e Tecnologia de Membrana, Campina Grande, Brasil, 8 - 11 de Julho de 2007, CD-ROM.

MULTI-OBJECTIVE DESIGN OF REACTIVE DISTILLATION

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*Computer-Aided
Chemical Engineering,
Vol. 24. Editors:
V. Plesu and P. S.
Agachi, Elsevier,
pp. 407-412.*

This work addresses the multi-objective design of complex reactive distillation columns. The concept of feasible regions is employed to investigate the use of internal reaction distribution, as well as superheated and subcooled feeds. We generate the Pareto surfaces relating the amount of reactive holdup, the number of stages and a cost indicator reflecting energy usage and column size. The most promising designs are identified and investigated further using rigorous simulations in Aspen Plus. A satisfactory agreement between approaches was found.

EFFECT OF PHYSICO-CHEMICAL PARAMETERS ON BIOCATALYSIS OF GLUCOSE 2-OXIDASE FROM *Coriolus versicolor* AT HIGH PRESSURE

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Glucose 2-oxidase (pyranose oxidase, pyranose:oxygen-2-oxidoreductase, EC 1.1.3.10) catalyses the oxidation of D-glucose at carbon 2 in the presence of molecular oxygen producing D-glucosone (2-keto-glucose; D-arabino-2-hexosulose) and hydrogen peroxide(1). This enzyme is of great importance since the reaction product (D-glucosone) is an important precursor for biosynthesis of the antibiotic cortalcerone. On the other hand, D-glucosone has been shown to exhibit anti-cancer activity *in vitro* against some cancer cell lines. The present work involves the conversion of D-glucose into D-glucosone in the presence of glucose 2-oxidase from *Coriolus versicolor* at high pressures with compressed air in a modified commercial reactor. The apparatus consists basically of one batch reactor (Micro Reactor Parr Instruments CO, 4843) with 25 ml of capacity equipped with agitation, temperature and pressure reading devices. Several parameters affecting biocatalysis at high pressures, up to 20 MPa, were investigated as follows: pressure, temperature, pH, enzyme concentration, enzyme immobilization and the presence of catalase. The conversion of D-glucose into D-glucosone in the presence of glucose 2-oxidase activity was investigated by using an HPLC system. The data presented in this work revealed an increase in the rate of reaction as a function of pH in the following order: pH 8.0 > pH 5.0 > pH 6.5 in the presence of catalase. The presence of catalase was found to increase the rate of conversion of D-glucose both at high pressures as well as at NTP with or without bubbling with pure O₂. The immobilized form of enzyme in a dialysis membrane exhibited about 50% of activity compared with the free enzyme and it could be re-used several times without a significant loss of enzyme activity.

Publicado em:
COST ACTION D30,
"High Pressure Tuning
of Chemical and
Biochemical
Processes", Bordeaux,
France.

POLIFENÓIS EM VEGETAIS DE USO TRADICIONAL NA COZINHA PORTUGUESA

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Publicado em:
Actas do 8º Encontro de Química dos Alimentos – Alimentos Tradicionais, Alimentos Saudáveis, Rastreabilidade, Escola Superior Agrária de Beja, Beja, 4 – 7 de Março de 2007, pp. 231 – 233.

A quantificação dos compostos fenólicos em extractos de couve galega, nabiça, acelga e rucola foi realizada por espectroscopia de absorção molecular no visível, segundo o método de Folin-Ciocalteu e recorrendo a uma curva de calibração com ácido gálico. A extracção dos polifenóis da matriz vegetal, fresca ou seca e previamente homogeneizada, foi realizada com etanol à temperatura ambiente e auxiliada através da aplicação de ultrassons. O teor em compostos fenólicos nos extractos das plantas frescas variou entre 16,8 e 8,8mgAG/g matéria seca, apresentando os extractos de couve galega e nabiça a concentração mais elevada e com valor semelhante. Nos extractos de rucola observou-se o menor teor em polifenóis enquanto que nos de acelga se determinou uma concentração média de $13,0 \pm 1,4$ mgAG/g matéria seca. A determinação dos compostos fenólicos nos extractos das amostras previamente sujeitas ao processo de secagem, conduziu a valores inferiores cerca de 70 a 80% aos determinados a partir das plantas frescas, com a excepção da rucola em que se observou uma redução de aproximadamente 45%.

PROCESSO DE PRÉ-EXPANSÃO DE CORTIÇA POR ACÇÃO DE VAPOR DE ÁGUA SATURADO E/OU SOBREAQUECIDO E PRODUTO RESULTANTE DO MESMO

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Proprietário: Amorim Isolamentos S.A., Mozelos, Portugal

Patente Número: 103698 R

Data de Apresentação Nacional: 21 de Março de 2007

A presente invenção apresenta um processo de pré-expansão por submissão da cortiça a vapor de água saturado ou sobreaquecido, capaz de promover a expansão da cortiça sem recurso a substâncias estranhas ao sistema cortiça. A expansão conseguida pelo processo de pré-expansão apresenta valores que podem atingir os 50%.

A expansão da cortiça por este processo de pré-expansão por submissão da cortiça a vapor de água saturado ou sobreaquecido é conseguida em qualquer material de cortiça independentemente da sua forma, origem, qualidade ou pré-tratamentos já realizados, portanto falca, cortiça virgem ou de reprodução, pranchas de cortiça, desperdícios de cortiça (resultantes do fabrico de rolhas ou da transformação de pranchas de cortiça), triturada, granulada ou em pó, quaisquer delas, cozida ou não cozida, resultando num novo material cortiça mas com propriedades melhoradas.

A presente invenção mostra também as alterações do novo material cortiça particularmente através do aumento do tamanho das células, da diminuição do peso específico e do aumento da tensão de ruptura e estabilidade dimensional dos aglomerados produzidos.

Publicado em:

Acta Crystallographica C, 2006, C62, m531-m534.

OS ULTRASSONS FOCALIZADOS NA EXTRACÇÃO DE METAIS EM AMOSTRAS AMBIENTAIS

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Publicado em:

Tendencias Actuales de la Ciencia del Suelo, N. Bellinfante & A. Jordán (eds.); 1ª edición, ISBN 978-84-690-4129-1, 2007, 648-657.

O presente trabalho compara a eficiência da extracção de metais tóxicos de uma amostra de solo, quando esta sofre um processo de digestão assistido por tecnologia de microondas e por tecnologia de ultrassons.

As amostras de solo estudadas foram recolhidas em diversos locais da cidade de Lisboa, e após um pre tratamento, foram submetidas aos processos de digestão utilizando água régia como reagente de extracção. O metal escolhido para o presente estudo foi o chumbo (Pb²⁺) e os resultados obtidos permitem verificar que em qualquer um dos locais investigados obtém-se uma maior recuperação deste metal quando as amostras de solo são sujeitas ao processo de digestão assistida por ultrassons.

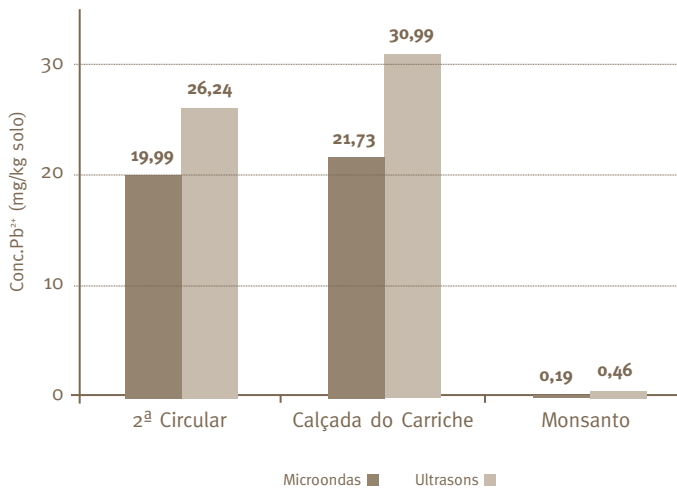
As amostras de solo recolhidas foram recolhidas em diversos locais da cidade de Lisboa (2ª Circular, Calçada do Carriche e Monsanto), segundo um processo de amostragem que visou uma caracterização o mais rigorosa possível de cada local [16], em termos da poluição pelo chumbo. As amostras foram digeridas com recurso quer à tecnologia de microondas quer à tecnologia de ultrassons, tendo sido utilizado como reagente de extracção a água régia (HCl 37%, Suprapuro, Merck; HNO₃ 65%; Suprapuro, Merck numa proporção de 3:1). O teor em chumbo foi determinado por Espectrometria de Absorção Atómica com Câmara de Grafite.

A preparação prévia das amostras de solo consistiu na secagem do solo em estufa, a 65°C, durante 96h, seguida de peneiração com aproveitamento da fracção igual e inferior a 2mm, trituração com um moinho de bolas até obter um pó tão fino quanto possível e pesagem de aproximadamente 2g de amostra para posterior digestão. O resíduo dos processos de digestão foi diluído a um volume final de 100 mL. Para peneiração das amostras de solo, após secagem, foi utilizado um sistema de peneiração Retsch AS 200 Control “g”. Para moagem das amostras foi utilizado um moinho de bolas de ágata Retsch S100. A digestão das amostras assistida por microondas foi efectuada num digestor de vaso aberto, série CEM Star System 2, com unidade lavagem de vapores de digestão. As digestões assistidas por ultra-

sons foram realizadas com uma cabeça de ultrasons Bandelin, Sonopuls GM 2200; sonda SH 219 G com ponta de titânio TT 19. Os ensaios de quantificação do chumbo por Espectrometria de Absorção Atômica foram efectuados com um espectrômetro de absorção atômica, série SOLAAR M5, equipado com atomizador de chama, câmara de grafite e pipetador automático. Os resultados obtidos na análise das várias amostras de solo, em termos de eficiência da recuperação do chumbo, de acordo com o tipo de processo de digestão utilizado, mostram-se na tabela abaixo:

Local	Concentração de Pb ²⁺ (mg/kg de solo)	
	Microondas	Ultrasons
Calçada do Carriche	21.73±2.74	30.99±2.63
2 ^a Circular	19.99±2.53	26.24±2.57
Monsanto	0.19±0.44	0.46±1.05

De acordo com os resultados que se mostram na tabela pode verificar-se que a digestão assistida por ultrasons conduz, invariavelmente, a uma maior eficiência em termos da extracção do chumbo da matriz da amostra.



DETERMINAÇÃO DO TEOR DE PGEs EM SOLOS RECOLHIDOS NA CIDADE DE LISBOA

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201-209.*

No presente trabalho procedeu-se à determinação dos teores de PGEs (Platinum Group Elements) presentes no solo de diversos locais da cidade de Lisboa, proveniente da utilização de catalisadores nos veículos automóveis. Este estudo foi realizado em seis locais da cidade, caracterizados por diferentes intensidades de tráfego automóvel, nos anos de 2003 e 2004. Em cada local foram recolhidas 12 amostras (a uma profundidade de 20cm) distribuídas através de três círculos concêntricos com raios de 1, 3 e 5m, segundo a direcção dos principais pontos cardeais. Prepararam-se amostras compostas de cada local por mistura das diversas amostras individuais. De cada amostra composta retiraram-se aproximadamente 2g que foram sujeitas a um processo de digestão ácida, assistida por tecnologia de microondas, e utilizando como reagente de digestão a água-régia.

A escolha dos locais de amostragem foi efectuada tendo em conta critérios como: a intensidade de tráfego automóvel, a densidade populacional, a existência de espécie indicadora e a topologia do local ao nível da maior ou menor dificuldade na dispersão dos poluentes. A quantificação dos PGEs foi efectuada por ICP-MS, verificando-se uma dependência directa entre os teores de PGEs determinados e a intensidade de tráfego automóvel nos locais analisados, precedida de um processo de optimização dos parâmetros operatórios.

Os resultados obtidos no presente trabalho permitem concluir que, em termos gerais, foram atingidos os principais objectivos inicialmente propostos, *a*) a optimização do processo de digestão ácida das amostras reais de solos de matriz complexa assistida por tecnologia de microondas, *b*) a optimização das condições de análise em GFAAS para posterior quantificação dos PGEs, *c*) a detecção e posterior quantificação dos metais em estudos (Pt, Pd e Rh) nos diversos locais da cidade de Lisboa por ICP-MS. Neste trabalho demonstrou-se também que amostras compostas são representativas dos vários pontos de amostragem, reduzindo assim o número de análises necessárias para a caracterização de um dado local. Este aspecto traduziu-se numa diminuição drástica do tempo global de análise. A platina, o paládio e o ródio existem no ambiente em teores mensuráveis, sendo

por isso importante a sua monitorização e quantificação, principalmente em meios urbanos. Os teores determinados são já significativos mostrando a origem antropogénica deste metal. Foi também possível estabelecer uma correlação entre os teores de PGEs e a intensidade de tráfego dos vários locais, demonstrando assim que o seu aparecimento está directamente relacionado com o tráfego automóvel.

Os resultados obtidos entre 2003 e 2004, permitem concluir que os níveis mais altos de PGEs registam-se no Marquês Pombal e na 2^a Circular. As principais razões para os elevados valores nesses locais são a elevada intensidade de tráfego a qualquer hora do dia, o facto do trânsito ser caracterizado por um tipo “Stop and Go”.

Com um perfil de trânsito “Stop and Go” o catalisador tem dificuldades em atingir as temperaturas ideais de funcionamento ($\cong 500\text{ }^{\circ}\text{C}$), tendo uma eficiência reduzida. Esse factor provoca uma erosão térmica e mecânica e os metais podem ser libertos para o meio ambiente sob a forma metálica ou sob a forma de sais halogenados, depositando-se nos solos ao longo dos anos.

No caso do Marquês de Pombal, este apresenta para além de uma elevada intensidade de tráfego automóvel uma topologia fechada não facilitando a dispersão dos metais existentes na atmosfera, acabando estes por se depositarem nos solos.

O paládio é o metal que se encontra em maiores quantidades nos solos, e uma possível explicação é a substituição da platina e/ou ródio pelo paládio, como elemento catalítico, em certas aplicações comerciais, de modo a reduzir os custos desses sistemas.

SOLUBILIDADE DE GASES EM ÁGUA E EM MEIOS DE FERMENTAÇÃO

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O livro apresenta o trabalho de pesquisa realizado pela autora no âmbito de sua tese de doutoramento em Engenharia Química na área da Solubilidade de Gases em Líquidos.

O estudo refere a determinação experimental da solubilidade de metano, etileno, propeno e 1-buteno em água e em meios de fermentação no intervalo de temperatura de 298,15 a 323,15K e à pressão atmosférica, num aparelho em vidro. A instalação experimental foi construída no Laboratório de Termodinâmica Experimental do Instituto Superior Técnico e utiliza o método de saturação, permitindo a determinação dos valores de solubilidade com uma precisão de $\pm 0,3\%$. O cálculo das solubilidades a partir das medidas experimentais envolveu métodos iterativos que se baseiam num tratamento termo dinâmico rigoroso cuja descrição é apresentada em detalhe neste livro.

Os valores de solubilidade do metano e etileno em água determinados neste estudo apresentaram uma boa concordância com os de maior rigor existentes na literatura. Relativamente ao propeno e 1-buteno os desvios encontrados já foram significativos. Nos meios de fermentação, os valores de solubilidade foram inferiores em cerca de 2,5% aos determinados na água no mesmo intervalo de temperatura. O estudo da variação da solubilidade dos diferentes gases com a temperatura permitiu determinar as funções termodinâmicas relativas ao processo de dissolução e discutir eventuais alterações estruturais em solução.

Nos últimos capítulos é descrita, em pormenor, a aplicação da *Scalped Particle Theory* e do modelo *UNIFAC* na previsão e correlação da solubilidade de gases em água.

REGRAS DE ORDENAMENTO A APLICAR EM INSTALAÇÕES DE SANEAMENTO BÁSICO E DE RESÍDUOS SÓLIDOS URBANOS

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Mestrado em: Ordenamento do Território e Planeamento Ambiental

Grau Concedido por: Faculdade de Ciências e Tecnologia da Univ. Nova de Lisboa

Orientadores: Maria da Graça Martinho

Provas Concluídas em: 4 de Outubro de 2006

Considerando cada vez mais a evidência e a necessidade de integrar os problemas ambientais no processo de ordenamento do território, pretendeu-se com este trabalho, definir regras de localização adequadas, do ponto de vista da sustentabilidade ambiental e de ordenamento territorial, aplicadas a Estações de Tratamento de Águas Residuais Urbanas e a Sistemas Integrados de Gestão de Resíduos Sólidos Urbanos. O intuito é minimizar os impactes ambientais decorrentes da sua laboração e má localização e a compatibilizar o uso do solo com estas funções. Um destaque especial para a utilização de uma ferramenta de trabalho muito importante nas questões ambientais, que é a Avaliação Ambiental Estratégica, a qual foi determinante na metodologia deste trabalho. Primeiramente, caracterizou-se, do ponto de vista legal e técnico - ambiental as referidas infra-estruturas, seguidamente, procedeu-se à recolha de informação relativa aos impactes ambientais que lhe estão associados, posteriormente, interpretaram-se os resultados obtidos essencialmente por entrevistas efectuadas às populações circundantes e pela aplicação de matrizes classificadoras desses mesmos impactes. Finalmente, foi proposto um conjunto vasto de regras de localização adequada para infra-estruturas de tratamento de águas residuais urbanas e de resíduos sólidos urbanos e, também, a sua integração em planos de ordenamento do território e em futuras versões dos planos estratégicos de águas residuais e de resíduos sólidos.

HIDROISOMERIZAÇÃO DE n-HEXANO SOBRE CATALISADORES BIFUNCAIONAIS À BASE DO ZEÓLITO BETA E MCM-22

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Provas Conduzidas em: 25 de Junho de 2007

Neste trabalho estudou-se o comportamento de catalisadores bifuncionais à base dos zeólitos MCM-22 e BEA na transformação de n-hexano.

Os zeólitos MCM-22 e BEA foram modificados a fim de preparar catalisadores bifuncionais por introdução de Pt usando diferentes métodos. Foram também introduzidos elementos de terras raras, La, Nd e Yb. Prepararam-se ainda catalisadores bi-metálicos Pt-Ni/BEA.

O conjunto de catalisadores foi caracterizado recorrendo às técnicas de difracção de raios-X, microscopia electrónica de varrimento e de transmissão, adsorção de azoto e de tolueno, adsorção de piridina seguida por espectroscopia de infravermelho, quimisorção de H₂, redução a temperatura programada com H₂ e reacções de *cracking* de n-heptano e hidrogenação do tolueno.

O modo de introdução da Pt no zeólito condiciona a localização das reacções que ocorrem, durante a transformação de n-hexano, no interior ou na superfície externa dos zeólitos, influenciando a actividade e selectividade, fundamentalmente no caso do zeólito MCM-22.

A presença de TR exerce um efeito conjunto na acidez e na função metálica dos catalisadores à base do zeólito BEA, manifestando-se sob a forma de um ligeiro aumento na selectividade em produtos bi-ramificados. Observou-se o mesmo efeito nos catalisadores bi-metálicos Pt-Ni/BEA, devido à interacção entre os dois metais.

UTILIZAÇÃO DE DERIVADOS DE CALIXARENOS NO ISOLAMENTO DE PROTEÍNAS E BIOCATÁLISE EM SOLVENTES ORGÂNICOS

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Provas Concluídas em: 15 de Dezembro de 2007

Neste trabalho foram utilizados ácidos carboxílicos derivados de *p-tert*-butilcalix[4,6,8]areno na extracção selectiva de duas proteínas: a mioglobina e a hemoglobina. Os três calixarenos apresentaram a capacidade de extrair as proteínas para a fase orgânica, com parâmetros de extracção superiores a 0,90.

Estas proteínas demonstraram pseudoactividade de peroxidase na reacção de oxidação da seringaldazina na presença de peróxido de hidrogénio, quer em meio aquoso quer em meio orgânico usando o derivado ácido de *p-tert*-butilcalix[6]areno em clorofórmio. A biocatálise destas duas proteínas foi investigada variando os seguintes parâmetros: pH, concentração da proteína e do substrato.

A actividade específica máxima da mioglobina foi determinada em meios aquoso e orgânico obtendo-se os valores de $1,08 \times 10^{-1}$ e $1,37 \times 10^{-1}$ U. mg proteína⁻¹ a pH inicial de 6,5, respectivamente. A hemoglobina apresentou em meio aquoso actividade específica máxima de 1,04 U. mg proteína⁻¹ a pH 5,5 e em meio orgânico de $9,92 \times 10^{-2}$ U. mg de proteína⁻¹, a pH inicial de 7,5.

Os parâmetros cinéticos em meio aquoso ($V_{m\acute{a}x}$, K_m , k_{cat} e k_{cat}/K_m) foram determinados em função do pH, assim como os parâmetros cinéticos aparentes ($V'_{m\acute{a}x}$, K'_m , k'_{cat} e k'_{cat}/K'_m) em meio orgânico.

A estabilidade do complexo proteína-calixareno foi analisada para ambas as proteínas em função do pH inicial tendo-se obtido valores de $t_{1/2}$ na gama de 2 – 5 dias. Os complexos proteína-calixareno no meio orgânico foram recuperados para soluções aquosas frescas alcalinas, com valores de recuperação da pseudoactividade de peroxidase superiores a 100%. O derivado ácido de *p-tert*-butilcalix[6]areno foi utilizado na extracção da hemoglobina a partir de sangue humano obtendo-se um valor de 0,50 para o parâmetro de extracção. A proteína foi purificada a partir de sangue humano usando uma matriz cromatográfica de um polímero contendo unidades de *p-tert*-butilcalix[6]areno na forma ácida, com um rendimento final de pseudoactividade da hemoglobina de 34,42% e um factor de purificação de 12. A análise electroforética da preparação purificada da hemoglobina revelou uma banda de proteína com Mr de 61kDa em PAGE nativa que foi coincidente com a banda de pseudoactividade de peroxidase *in situ*.



05

ENGENHARIA DE SISTEMAS DE POTÊNCIA E AUTOMAÇÃO

Anuário Científico 2007

ISEL

A LOW-COST, ACCURATE AND NON-INTERCEPTING CONTINUOUS METHOD FOR BEAM CURRENT MEASUREMENTS IN A HIGH-CURRENT ION IMPLANTER

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The development of a low cost, accurate, non-intercepting continuous method, for measuring the beam current in the High Current Ion Implanter, at the Nuclear and Technological Institute (ITN), Sacavém (Portugal), is described. The developed method, here named Differential Current Monitor (DCM), is based on the electric charge conservation principle, applied to the electric currents that flow in the implanter electrical system, due to the acceleration voltage applied to the ion beam and the leakage currents to ground. This method allows for the continuously ion beam current measure without intercepting it to the target. Since its installation, it is possible to accurately measure ion beam currents from tens of μA to mA, which are the normal ion current range, for this type of implanting systems, depending on the ion mass. The ion current measurements precision is determined by calculating the implanted dose by RBS (Rutherford Back Scattering). In addition, this method enables the performance evaluation of the high voltage power supplies and the leakage resistors that control the applied voltages in the implanter.

Publicado em:

Nuclear Instruments and Methods in Physics Research Section B, (2007), Volume 265, Issue 2, pp. 576-580.

PULSE SHAPE IMPROVEMENT IN CORE-TYPE HIGH-VOLTAGE PULSE TRANSFORMERS WITH AUXILIARY WINDINGS

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Nowadays, high-voltage pulsed power based technologies are rapidly emerging as a key to efficient and flexible use of electrical power for many industrial applications. One of the most important elements in high-voltage pulse generating circuit technology is the transformer, generally used to further increase the pulse output voltage level. However, its non-ideal behavior has significant influence in the output pulse shape.

In spite of all winding and switching techniques, the most attractive winding configuration for high-voltage, the core type transformer with primary and secondary on different core legs, is seldom used in pulsed applications, due to the weak magnetic coupling between windings, which would result in a slow rising output voltage pulse.

This paper shows that auxiliary windings, suitably positioned and connected, provide a dramatic improvement in the pulse rise time in core type high-voltage pulse transformers. A mathematical model is derived and used to describe the observed behavior of the transformer with auxiliary windings. The model is discussed regarding the experimental results, obtained from a high-voltage test transformer associated with a high-voltage pulse generating circuit, and the simulation results obtained from the numerical evaluation of the developed differential equations implemented in Matlab considering the measured transformer parameters.

Publicado em:

*IEEE Transactions on
Magnetics, vol. 43,
no. 5, May 2007,
pp. 1973-1982.*

ANALYSIS OF A MODULAR GENERATOR FOR HIGH-VOLTAGE, HIGH-FREQUENCY PULSE APPLICATIONS, USING LOW VOLTAGE SEMICONDUCTORS (<1kV) AND SERIES CONNECTED STEP-UP (1:10) TRANSFORMERS

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This paper discusses the operation of a modular generator topology, which has been developed for high-frequency (kHz), high-voltage (kV) pulsed applications. The proposed generator uses individual modules, each one consisting of a pulse circuit based on a modified forward converter, which takes advantage of the required low duty cycle to operate with a low voltage clamp reset circuit for the step-up transformer. This reduces the maximum voltage on the semiconductor devices of both primary and secondary transformer sides. The secondary winding of each step-up transformer is series connected, delivering a fraction of the total voltage. Each individual pulsed module is supplied via an isolation transformer.

The assembled modular laboratorial prototype, with three 5kV modules, 800V semiconductor switches and 1:10 step-up transformers, has 80% efficiency, and is capable of delivering, into resistive loads, -15kV/1 A pulses with 5 μ s width, 10kHz repetition rate, with less than 1 μ s pulse rise time. Experimental results for resistive loads are presented and discussed.

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*Review of Scientific
Instruments* 78,
034702, 2007.

MODULAR PULSED GENERATOR FOR kV AND kHz APPLICATIONS BASED ON FORWARD CONVERTERS ASSOCIATIONS

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The operation of a modular generator topology, developed for kHz and kV pulsed applications, is presented. The proposed generator uses individual modules each one consisting of a pulse circuit based on a modified forward converter topology, with the secondary windings series connected, delivering a fraction of the total voltage. A laboratorial prototype with three 5kV modules, 800V semiconductor switches and 1:10 step-up transformers has been assembled. The first experimental results of this modular generator are presented and discussed. The circuit has 80% efficiency and is capable of delivering, into resistive loads, -15kV/1 A pulses with 5 μ s width, 10kHz frequency, with less than 1 μ s pulse rise time.

Publicado em:

Conference Proceeding of the, 12th European Conference on Power Electronics and Applications, 2-5 September 2007, Aalborg, Denmark, pp. 1-7.

REPETITIVE ALL-SOLID-STATE PULSE MARX TYPE GENERATOR WITH ENERGY RECOVERY CLAMP CIRCUIT FOR INDUCTIVE LOADS

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A newly developed Marx type circuit topology that achieves both output-voltage multiplication and energy recovery, which has been developed for inductive load applications, namely Electromagnetic metal Forming (EMF), based on an all-solid-state Marx type generator, is described.

The proposed circuit takes advantage on the power semiconductor switches intensive use, replacing the conventional Marx Bank passive elements, to increase the performance, strongly reducing losses and increasing the pulse repetition frequency. Additionally, the generator is designed with an energy reset circuit that enables the use of inductive loads, recovering the inductive energy during the semiconductor switches off-state, back to the energy storage capacitors. Preliminary results from this EMF modulator prototype are presented and discussed.

Publicado em:

Conference Proceedings, 34th IEEE International Conference on Plasma Science and the 16th IEEE International Pulsed Power Conference June 17-22, 2007, Albuquerque, New Mexico.

SOLID-STATE MARX GENERATOR DESIGN WITH AN ENERGY RECOVERY RESET CIRCUIT FOR OUTPUT TRANSFORMER ASSOCIATION

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In this paper the circuit topology of a hybrid fully integrated solid-state Marx generator circuit, developed for kHz and kV applications, is presented and analysed. The proposed circuit uses only power semiconductor switches to increase the performance, being designed with a magnetizing energy reset circuit that enables the use of an output pulse transformer, which recovers the transformer magnetizing energy during the off switches state, back to the energy storage capacitors. This enables higher frequency operation, increasing the pulse generator yield.

A 10kHz pulse rate laboratory prototype with five stages was built using 1200V IGBTs and diodes. Experimental results show almost rectangular pulses with -5kV, 4 to 10 μ s width, into a 5 k Ω resistive load.

Publicado em:

*Conference
Proceedings, 38th IEEE
Power Electronics
Specialists Conference,
17-21 June 2007,
Orlando, EUA,
pp. 2987-2991.*

ISOLATED AUTONOMOUS CAPACITIVE POWER SUPPLIES FOR TRIGGER FLOATING SEMICONDUCTORS IN A MARX GENERATOR

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This paper reports the development of isolated autonomous capacitive power supplies to charge each drive circuit of the high voltage floating semiconductor stage in a solid-state Marx Generator. The circuit takes advantage of an auxiliary capacitor, charged in series with the main energy storage capacitor in each Marx generator stage, to supply the optic-fibre isolated gate drive circuit of the solid state switches. Laplace domain circuit analysis is made to determine the values of these capacitors and to obtain the desired voltages, with low ripple, for the required load. A laboratory prototype with three stages, 3kW peak power, of this all silicon Marx generator circuit, with optic-fibre isolated triggering signals and autonomous capacitor isolated charging power supplies was built using 1200V IGBTs and diodes, operating with 1000V d-c input voltage and 10kHz frequency, giving 3kV and 10 μ s pulse with, approximately, 15V isolated autonomous power supplies in each stage.

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*Conference
Proceedings, IEEE
International
Symposium on
Industrial Electronics",
4-7 June Vigo/Spain,
2007, pp. 821-826.*

FORECASTING THE IMPACT OF INCREASING INTEGRATION OF RENEWABLE SOURCES IN THE POWER UNBALANCE DURING PEAK AND OFF-PEAK HOURS

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Environmental impacts and external dependency associated with energy consumption can be minimized with integration of renewable power sources. Portugal, as well as a number of other countries, presents a sharp increase in renewable sources integration, namely in power sources like wind, solar photo-voltaic, waves, biomass and small hydro.

As all renewable technologies ultimately derive energy from natural sources that vary in their availability over different time-scales, the integration of larger amounts of renewable sources will become an increasingly important issue for the balancing of power generation and demand.

The main objectives of this paper is to present a forecast methodology to quantify power generation and demand unbalance and characterize that sort of unbalance, specially focusing peak and off-peak periods' specificities.

Heeding the distinction between peak and off-peak hours, the results obtained show that the unbalance compartment is particularly distinct in these periods, namely with generation shortage in peak hours and excess of generation in off-peak hours.

ESTIMATING FUTURE POWER GENERATION UNBALANCE IN THE PORTUGUESE POWER SYSTEM DUE TO INCREASING INTEGRATION OF RENEWABLE SOURCES

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Integration of renewable sources in energy production avoid the use of fossil sources, which are responsible for great environmental impacts and excessive dependency of energy imported products. However, increasing integration of renewable sources in a power system can introduce some new issues in its operation, such as potential unbalancing between generation and demand, especially in off-peak periods with high levels of hydro generation. This paper presents an estimate of the future power generation unbalance in the Portuguese power system due to increasing penetration of renewable sources.

Publicado em:

Proceedings of the International Conference on Power Engineering, Energy and Electrical Drives – Powereng 2007, Setúbal, 12-14 April, 2007.

CONTRIBUTION OF ENERGY STORAGE SYSTEMS FOR POWER GENERATION AND DEMAND BALANCING WITH INCREASING INTEGRATION OF RENEWABLE SOURCES: APPLICATION TO THE PORTUGUESE POWER SYSTEM

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Increasing integration of renewable sources introduce some new issues on the operation of the power system, such as potential unbalancing between generation and demand, especially in off-peak periods with high levels of hydro generation. This scenario can get worse when associated with the installation of a nuclear powerplant, which operates on a must run basis. This paper analyses the contribution of energy storage systems use to avoid future power generation and demand unbalance in the Portuguese power system. Moreover it is also presented an overview of the available energy storage technologies and the role of power electronics on its appropriate operation.

Publicado em:

Proceedings of the 12th European Conference on Power Electronics and Applications – EPE 2007, Aalborg, Denmark, 2-5 September, 2007.

FUZZY CONTROLLER FOR AUTOMATIC ADJUSTEMENT OF THE ELECTROMECHANICAL POSITION DRIVE TRAJECTORY

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This paper describes the development of a methodology to synthesize fuzzy controllers to correct the tracking dynamics of an electro-mechanical positioning drive trajectory.

A brief introduction to tubular linear synchronous motors is presented. Special focus is made on parallel manipulators using tubular linear synchronous permanent magnet motors, where computer simulations confirmed large amplitude variations of load forces applied to linear actuators of an existing six degrees of freedom (6 DOF) parallel manipulator.

The fuzzy controller synthesis for the linear position drive is described. Its main goal is to perform the automatic adjustment of the tubular linear motor positioning trajectory, by changing its speed and acceleration references. The laboratory prototype and the experimental results of the fuzzy controller coupled to the electromechanical linear position drive are presented and discussed.

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*CEE'07 – 2nd
International
Conference on
Electrical Engineering,
Coimbra, 26 a 28 de
Novembro, pp. 15.*

FUZZY CONTROLLER FOR AUTOMATIC ADJUSTEMENT OF THE ELECTROMECHANICAL POSITION DRIVE TRAJECTORY

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Publicado em:
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International
Conference on
Electrical Engineering,
Coimbra, 26 a 28 de
Novembro, pp. 15.

This paper describes the development of a methodology to synthesize a fuzzy controller to correct the tracking dynamics of the electro-mechanical positioning drive trajectory.

A general framework about topologies in the field of linear electro-mechanical drives is presented. Special focus is made on parallel manipulators using tubular linear synchronous permanent magnet motors, where computer simulations confirmed large amplitude variations of load forces applied to linear actuators of the six degrees of freedom (6 DOF) parallel manipulator. The 6 DOF parallel manipulators are wide used for the support of the flight simulators, and are projected to emulate the aeronautic motions. The commercial 6 DOF parallel manipulators usually employ hydraulic linear actuators.

The hydraulic linear actuators have bigger volume/power ratio than tubular linear synchronous motors and an expensive maintenance cost. The difficulties of these applications are in the absence of the trajectory planning, which is common in parallel manipulator applications.

The fuzzy controller synthesis for the linear position drive is described. Its main goal is to perform the automatic adjustment of the tubular linear motor positioning trajectory, by changing its speed and acceleration references. The resulting motion trajectory obtained from the fuzzy controller is particularly suited to high accuracy applications such as parallels manipulators, robotics systems and factory automation.

The electromechanical position drive present in this paper is based on Permanent Magnet Tubular Linear Synchronous Motor (PM-TLSM) as the electromechanical linear actuator fed by a position drive controller and a linear encoder as feedback device of the system. The structure of the laboratory prototype of the fuzzy controller coupled to the electromechanical linear position drive is presented.

The experimental results demonstrate that the trajectory correction is made lower than 1s.

Comparing the experimental results with different loads, it is verified

that the position errors values does not depend of the load force applied to the tubular linear motor shaft.

The experimental results obtained are used to evaluate the performance of the fuzzy controller, which was able to reduce the positioning errors from 40% to 10%.

INVERSE KINEMATICS OF A 6-6 ELECTROMECHANICAL GOUGH-STEWART PLATFORM

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Gough-Stewart platforms (GS) are variable length octahedral hexapods, with 6 DOF. They are usually used in motion simulation and control area. In the GS platform referred in this paper the variable length legs are driven by electromechanical motors. The GS platform is a parallel manipulator which requires complex kinematics and dynamic studies due to its architecture, being the direct kinematics model often obtained using some mathematical simplifications. In this paper a theoretical study of the inverse kinematics is presented.

Publicado em:

*Proceedings of the
2nd International
Conference on
Electrical Engineering
(CEE'07). ISBN 978-
972-99064-4-2, p 124-
127, (in CD-ROM).
Coimbra, Portugal,
Nov. 26-28, 2007.*

ELECTROMECHANICAL GOUGH-STEWART PLATFORM ANALYSIS

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This paper addresses kinematics and dynamics of an electromechanical Gough-Stewart platform. A dynamic model of the electromechanical Gough-Stewart platform is implemented in simulation software and validated. A controller for the electromechanical Gough-Stewart platform is proposed and the dynamic response to some leg movements is analysed.

Publicado em:

Actas Y Congresos of the 2nd Seminar for Advanced Industrial Control Applications (SAICA 2007). ISBN 978-84-362-5519-5, p 155-161, Madrid, Spain, Nov. 5-6, 2007.

DESIGN OF IMPROVED RAIL-TO-RAIL LOW-DISTORTION AND LOW-STRESS SWITCHES IN ADVANCED CMOS TECHNOLOGIES

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Publicado em:
IEEE Proc. ICECS'07,
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pp 218-221.

Present and emergent CMOS technologies point to the use of low supply voltages. Special care and requirements are mandatory to guarantee that the linearity of the switches in the signal path is kept over rail-to-rail signal swings, needed in many low-voltage switched-capacitor circuits, spanning from 10-14b ADCs to accurate analog filters. On the other hand, the reliability constraints of the technology have to be considered, avoiding over-stress of the CMOS devices if large voltages are applied to the gates of the transistors. This paper addresses these challenges, using a simple SC linearization control circuit (SLC) that generates suitable gate control voltages when very low distortions are targeted, within the technology limits, to drive a CMOS transmission-gate. Exhaustive corner simulation results of a practical sample-and-hold circuit show that, using the proposed circuit, linearity/distortion levels above 12-bits can be reached over the entire Nyquist band. The proposed improved new circuit can be readily used in any advanced CMOS technologies for boosting the linearity of low-voltage high-swing CMOS switches.

PREDICTIVE OPTIMAL CONTROL OF INPUT AND OUTPUT CURRENTS IN MATRIX CONVERTERS

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This paper presents predictive optimal control concepts applied to the input and output current control in matrix converters. Given the converter non-linearity, the method uses a discrete-time model of the converter system to predict the future values of the output and input current for all the 27 possible output voltage vectors generated by the matrix converter. The optimal controller minimizes output and input current errors using a cost functional employing adequate weights. The performance of the proposed predictive control is validated by numerical simulation results, which are also compared with *Venturini* modulation.

Publicado em:

*Conferência
International
Conference on Power
Engineering, Energy
and Electrical Drives,
Setúbal, Portugal, de
12 a 14 de Abril de
2007.*

PREDICTIVE OPTIMAL CONTROL OF UNITY-POWER-FACTOR MATRIX CONVERTERS USED IN FIELD ORIENTED CONTROLLED INDUCTION MOTOR DRIVES

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This paper presents predictive optimal control applied to field oriented controlled induction machine drives employing a matrix converter with input current control and near unity input power factor. The method uses a discrete-time model of the converter system to predict the future values of the output and input currents for all the 27 possible output voltage vectors generated by the matrix converter. The optimal controller minimizes output current (allowing the establishment of field oriented control) and input current errors using a cost functional with adequate weights. The performance of the proposed predictive control is validated by numerical simulations, which are also compared to *Venturini* modulation.

Publicado em:

*Conferência
International
Symposium on
Industrial Electronics,
Vigo, Espanha, de 4 a
7 de Junho de 2007.*

THE USE OF THE SIFTING PROPERTY AND THE GENERALIZED DERIVATIVE TO CALCULATE FOURIER COEFFICIENTS

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This paper presents an educational approach for teaching how to calculate the Fourier coefficients of a periodic function by using the concept of generalized derivative and the sifting property of impulses. Calculation by hand of Fourier series of some periodic functions should be exercised before proceeding to the use of computational tools so widespread nowadays. Calculation by hand, usually a painstaking task, can be alleviated by providing efficient methods. The method proposed in this paper is easily understood by undergraduate and makes hand calculation of Fourier coefficients for partially continuous and periodic functions easy to perform in class.

Publicado em:

*Proceedings of the 18th
EAEEIE Annual
Conference Innovation
in Education for
Electrical and
Information
Engineering, Praga
(República Checa),
2 a 4 de Julho de
2007.*

ON EMISSIONS ECONOMIC DISPATCH: AN INNOVATIVE TEACHING

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This paper deals with important decisions that a generation company has to make for allocation of power systems fossil-fired units, regarding economic and emission operation.

A bi-objective optimization problem is proposed for modeling that operation in what regards teaching the most important aspects of the technical operation.

An innovative insight over the all range of the feasible electric power is presented, conveying the teaching of decisions on the dispatch of fossil-fired units.

Publicado em:

*Proceedings of the 18th
EAEEIE Annual
Conference Innovation
in Education for
Electrical and
Information
Engineering, Praga
(República Checa), 2 a
4 de Julho de 2007.*

A MICROCONTROLLER SENSORLESS SPEED CONTROL OF A DIRECT CURRENT MOTOR

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It is described a sensorless direct current motor drive. The speed was controlled using sliding mode with a first- order differential equation based on the speed error. The result of the switching function was integrated with a current limitation using a logic equation. The current limitation assures the machine protection and the output of the logic block is the signal of the voltage to apply on the motor armature. Instead to measure the rotor speed it was analytically inferred an external torque and speed observer. The motor is fed by a classic insulated gate bipolar transistor converter module. All gating signals for power switches are determined at every sample instant by a single microcontroller, which collects information and analyze voltage and current data from the motor to perform the necessary speed and torque estimation.

Publicado em:

ISIE 2007. Proceedings of the IEEE International Symposium on Industrial Electronics, 2007. Vigo, Espanha de 4 a 7 de Junho de 2007, pp 1143-1146, ISBN: 978-1-4244-0755-2.

A SENSORLESS TORQUE CONTROLLER TO A DIRECT CURRENT MOTOR DRIVE

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The external torque of a direct current motor is controlled using sliding mode with a first-order differential switching function based on the torque error whose result is integrated with a current limitation using a logic equation. The current limitation assures the machine protection and the output of the logic block determines the voltage signal to apply on the motor armature.

The external torque and the rotor speed are analytically inferred by a double observer whose inputs are the voltage and the current armature.

The obtained drive can be used to wind paper, wires or cables. The traction strength is controlled with a torqueless (and tacholeless) operation.

Publicado em:

*II CIEM2007, Actas do
II Congresso
Internacional de
Engenharia Energética
e Meio Ambiente.
Badajoz, Espanha de 6
a 8 de Junho de 2007,
ISBN: 978-84-96560-
45-1.*

PERFORMING KNOWLEDGE INTEGRATION WITH POWER ELECTRONICS DIDACTIC MODULES

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At ESTSetúbal, the engineering courses have an organization based on curricular units. In order to increment the knowledge integration, at the Electrical Engineering course, were implemented some multidisciplinary projects along the three years of the course.

Preliminary results shows that the students working on these projects are, in general, more motivated. It is possible to verify also that, with this methodology, the desired competencies of the course are more easily acquired. Some of these projects consist in the development of didactic modules, which will be used by other students.

Publicado em:

*Proceedings of the 18th
EAEEIE Annual
Conference, Innovation
in Education for
Electrical and
Information
Engineering (EIE).
Praga, República
Checa, de 2 a 4 de
Julho de 2007, ISBN:
978-80-01-03745-4.*

THE CO₂ PASS-THROUGH TO ELECTRICITY PRICES IN THE SPANISH ELECTRICITY MARKET

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Publicado em:

Proceedings da 4.^a Conferência Internacional "The European Electricity Market, EEM 07" – Challenge of the Unification, Cracóvia, Polónia, 23 a 25 de Maio de 2007.

The Spanish electricity pool prices increased significantly in 2005 in comparison with 2004.

Two main drivers that influence market prices are strategic behavior of market players and generation costs, which includes fuel costs and CO₂ emission costs.

This paper presents a study on the Spanish electricity market based on a conjectural variations model using the SiMEC market simulator. This study is intended to quantify the distinct impact of the strategic behavior of market players and the CO₂ pass-through to market prices in the increase of prices that occurred in 2005.

The results obtained show that the Spanish market players have not only passed the CO₂ emissions costs to electricity prices but also became less competitive in 2005.

In fact, according to the methodology used in this work to isolate the different drivers of the price increase, it was concluded that the 92% increase in pool prices from 2004 to 2005 are due to CO₂ pass-through in 40%, to the strategic behavior of market players in 18% and other factors such as demand, fuel prices and non thermal production in 34%.

FORECASTING THE BEHAVIOUR OF THE SOUTH AFRICAN ELECTRICITY MARKET USING AN OLIGOPOLISTIC GAME THEORETIC SIMULATOR

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In this paper we forecast the behaviour of the South African electricity market using an oligopolistic game theoretic simulator based on a conjectural variations model. For different market structures and for a given competitive regime, we simulate the South African electricity market. We compare prices, power production, profits, costs and incomes for the overall market, among those different market structures. We draw conclusions on the impact of the structure adopted on the incentives of the players to increase prices in order to maximize profits.

Publicado em:

Proceedings da 7ª Conferência Internacional "Power System Operation and Planning" ICPSOP 2007, University of Cape Town, South Africa, 22 a 25 de Janeiro de 2007.

A COMPARATIVE STUDY OF MARKET BEHAVIORS IN A FUTURE SOUTH AFRICAN ELECTRICITY MARKET

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This paper presents a comparative study on market behaviors in a proposed South African electricity market using two market simulation software, in order to evaluate different market structures and competition models. The results show that the design of market structure is essential to ensure proper competition. Market structure plays an important role on the determination of market clearing price and production. The more concentrated the market will result in higher market price. Overall profits in the market also vary with the change of market structure and competition models.

Publicado em:

Proceedings da Conferência Internacional "Power Tech 2007", Lausanne, Suíça, 1 a 5 de Julho de 2007.

HOW MARKET PLAYERS ADJUSTED THEIR STRATEGIC BEHAVIOUR TAKING INTO ACCOUNT THE CO₂ EMISSION COSTS - AN APPLICATION TO THE SPANISH ELECTRICITY MARKET

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This paper addresses the problem of the strategic behaviour of the power companies taking into account the CO₂ emission costs. The proposed methodology is applied to the Spanish electricity market, where the degree of competition, measured by the conjectural variation parameter of each market player, is computed for the first year of the European Union Emission Trading Scheme and compared to the previous year. For that purpose the SiMEC – SiMulator for Electricity and Carbon markets is used. From the results obtained it is concluded that the Spanish market players presented a less competitive behaviour in 2005 than in 2004, which means that the observed increase in prices are caused not only by the increase in fuel prices, dry conditions, CO₂ and other cost factors, but also by the strategic behaviour of the market players.

Publicado em:

Proceedings da 4^a Conferência Internacional "The European Electricity Market, EEM 07" – Challenge of the Unification, Cracóvia, Polónia, 23 a 25 de Maio de 2007.

ACPOWER CONCEPTS: USING A WORLDWIDE CONTROVERSY TO QUESTION CONCEPTS AND DEFINITIONS

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Non active power concepts used in electric power systems (namely reactive power, distortion power, apparent power and power factors) have been under debate for almost one century. Since there are still no consolidated definitions, the presentation of this kind of subject motivates a refreshment on critical reasoning about concepts and definitions in general. This kind of theoretical debate may be beneficial especially in a field dominated by consolidated theories and axiomatically structured explanations. After a brief historical review of the subject, the validity of different points of view are discussed taking into account a number of practical and logical requirements for establishing concepts in science and engineering. Suggestions are given on how the underlying controversy can be explored to stimulate active learning at a graduate level.

Publicado em:

*Proceedings of the 18th
EAEEIE (European
Association for
Education in Electrical
and Information
Engineering)
Conference, Praha,
2007.*

Actas em Conferência Nacional

APPLICATION OF PM TUBULAR LINEAR MOTOR DRIVE AS THE ELECTROMECHANICAL LINEAR ACTUATOR OF A 6 DOF PARALLEL MANIPULATOR

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² Dept. of Electrical and Computer Engineering, IST, Lisbon, Portugal

This paper describes the study of Permanent Magnet Tubular Linear Synchronous Motor (PM-TLSM) as the electromechanical linear actuator of a Six Degree of Freedom (6 DOF) Parallel Manipulator. The dynamic models of the PM-TLSM and the position drive controller are derived and implemented in Matlab in order to obtain simulation results to evaluate the dynamic response. The experimental results of the electromechanical linear positioning drive are presented and discussed to validate the mathematical model.

Publicado em:

*Engenharias'07 –
inovação &
desenvolvimento,
UBI - Covilhã,
21 a 23 Novembro
de 2007.*

DESENVOLVIMENTO DE UM CONTROLADOR FUZZY PARA UM POSICIONADOR ELECTROMECHANICO LINEAR

Luís, Ricardo Jorge Ferreira

Mestrado em: Engenharia Electrotécnica e Computadores

Grau Concedido por: Universidade Técnica de Lisboa

Orientadores: Doutor José Fernando Alves da Silva e

Doutor José Carlos Lourenço Quadrado

Provas Concluídas em: 20 de Julho de 2007

Descreve-se a metodologia de desenvolvimento de um controlador *fuzzy* para correcção do comportamento dinâmico no seguimento da trajectória de um posicionador electromecânico linear.

Apresenta-se uma perspectiva geral sobre as topologias, concepção e algumas aplicações relevantes no campo dos accionamentos electromecânicos lineares com particular ênfase ao accionamento de manipuladores paralelos com motores lineares tubulares. Comprova-se, através da simulação computacional, a grande amplitude de variação das forças de carga aplicadas aos actuadores electromecânicos lineares de um manipulador paralelo de seis graus de liberdade.

Desenvolve-se o modelo do posicionador electromecânico linear considerado neste trabalho e apresentam-se resultados de simulação numérica que permitem caracterizar o seu desempenho dinâmico.

Descreve-se a síntese do controlador *fuzzy* para o posicionador electromecânico linear, cujo objectivo é realizar a correcção automática do comportamento dinâmico de seguimento da trajectória de posicionamento do motor linear tubular, com base na alteração das suas referências de velocidade e aceleração. Apresentam-se os resultados de simulação numérica para o controlador desenvolvido.

Apresenta-se a estrutura global de implantação do controlador *fuzzy* para o posicionador electromecânico linear e procede-se à sua validação, com base nos resultados experimentais obtidos do seu funcionamento, verificando-se que os erros de posição são reduzidos pelo menos de 40% para 10%.

AUTOMATIZAÇÃO DE UM ACELERADOR DE PARTÍCULAS

Silva Lopes, José Gabriel da

Mestrado em: Engenharia Electrotécnica e de Computadores

Grau Concedido por: Instituto Superior Técnico

Orientadores: Doutor Francisco André Corrêa Alegria e

Doutor Luís Manuel dos Redondo

Provas Concluídas em: 17 de Julho de 2007

Nesta dissertação aborda-se a automatização da operação do acelerador de partículas do tipo “*Van de Graaff*” instalado no Laboratório de Feixes de Iões do Instituto Tecnológico Nuclear. Esta máquina, especialmente orientada para investigação na área da caracterização de materiais com base em técnicas de física nuclear, permite a produção de feixes de iões positivos de Hélio (He^+) e Hidrogénio (H^+) com energias até 3 MeV e intensidades de corrente de alguns microamperes. Para realizar o sistema automático utilizou-se um computador pessoal equipado com uma placa de aquisição de dados da *National Instruments*, módulos electrónicos e um software apropriado (LabVIEW). Para o efeito, foi necessário proceder-se ao estudo pormenorizado de todos os procedimentos de funcionamento, que tiveram de ser traduzidos para algoritmos matemáticos de forma a serem automatizados.

Adicionalmente, foi necessário proceder-se à adaptação de todos os sinais, ou variáveis, presentes no acelerador, para poderem ser passados através de uma placa de aquisição de dados para posterior tratamento informático.

Com o sistema a funcionar em automático, é possível controlar a operação do acelerador desde a aplicação de uma tensão de aceleração ao terminal, a formação dum plasma na fonte de iões, até à focagem de um feixe de iões de He ou H no alvo com a intensidade de corrente desejada.

Deste modo, reduz-se a necessidade de pessoal técnico especializado na operação da máquina permitindo, ainda, expandir a sua utilização a mais utilizadores sem formação especializada nos procedimentos do acelerador.

COMPENSAÇÃO DE ENERGIA REACTIVA COM CONVERSOR MULTINÍVEL TRIFÁSICO

Encarnação, Luís José Lamy Rocha da

Mestrado em: Engenharia Electrotécnica e de Computadores

Grau Concedido por: Instituto Superior Técnico

Orientadores: Doutor José Fernando Alves da Silva e

Doutor Vasco Emanuel Alves da Silva

Provas Concluídas em: 23 de Outubro de 2007

Este trabalho pretende dar um contributo para o desenvolvimento de novos sistemas de compensação de potência reactiva, de uma forma contínua e automática, em sistemas trifásicos sem neutro. Os sistemas de compensação de potência reactiva mais usuais são constituídos por associações de baterias de condensadores colocadas em paralelo com as cargas. Estes bancos de condensadores apresentam apenas alguns valores de capacidade, não têm possibilidade de compensar potências reactivas em cargas capacitivas e a entrada em funcionamento de um escalão de condensadores provoca uma distorção transitória na onda de tensão, afectando desta forma a qualidade de energia.

Propõe-se a criação de um sistema de compensação de energia reactiva usando conversores multinível trifásicos controlados por processador digital de sinal. É efectuada a modelação, o controlo e a simulação do sistema em estudo. Os resultados experimentais obtidos validam o estudo efectuado bem como mostram insensibilidade a variações de carga. Neste trabalho, salienta-se a aplicação da teoria da potência instantânea $p-q$, assim como a técnica de controlo por modo de deslizamento (*sliding mode control*). Neste tipo de controlo incorpora-se a técnica para equilibrar as tensões contínuas dos condensadores da alimentação do conversor multinível, sem recurso a meios exteriores.

Palavras-chave: Compensação de energia reactiva, controlo por modo de deslizamento, conversão multinível, modelação, electrónica de potência, teoria da potência instantânea $p-q$.

ESTUDO DE UMA PLATAFORMA ELECTROMECHANICA DE GOUGH-STEWART

Murta Pereira, Rita Marcos Fontes

Mestrado em: Engenharia Electrotécnica e de computadores

Grau Concedido por: Instituto Superior Técnico

Orientadores: Doutor José Fernando Alves da Silva e

Doutor José Carlos Lourenço Quadrado

Provas Concluídas em: 27 de Outubro de 2007

As plataformas de Gough-Stewart são estruturas hexapódicas octaédricas que possuem seis graus de liberdade, em que as seis pernas têm comprimento variável. O seu domínio de aplicação enquadra-se, de modo geral, em simuladores de movimento.

A plataforma de electromecânica de Gough-Stewart consiste num manipulador paralelo com seis graus de liberdade cujo modo de accionamento é electromecânico. Pelas suas características de estrutura mecânica, a plataforma de Gough-Stewart necessita de estudos de cinemática e de dinâmica relativamente complexos. Para a obtenção da cinemática directa é frequente encontrarem-se estudos baseados nalgumas simplificações. Os estudos que permitem caracterizar a dinâmica da plataforma de Gough-Stewart estão significativamente menos desenvolvidos quando comparados com os estudos da sua cinemática.

Apresenta-se neste trabalho o enquadramento da plataforma electromecânica de Gough-Stewart no contexto actual dos estudos existentes neste domínio.

Estuda-se a cinemática da plataforma electromecânica. Apresenta-se a cinemática directa recorrendo à aproximação da plataforma de Gough-Stewart do tipo 6-6 a uma plataforma de Gough-Stewart do tipo 6-3. Apresenta-se e valida-se o modelo da dinâmica da plataforma de Gough-Stewart. Dimensiona-se um controlador possível para a plataforma electromecânica de Gough-Stewart e estuda-se o seu comportamento dinâmico por simulação.



FÍSICA

Anuário Científico 2007

ISEL

INSTABILITIES IN LIQUID FOAMS

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Instabilities play a central role in the physics of foams. Some that change the topology of a dry foam are indicated by the laws promulgated by Plateau in his 1873 book. Their occurrence is less clearly predictable in wet foams. Various other instabilities are related to gravitational loading and gas compressibility. We gather up many examples as a guide to future research and identify problems that remain, including what we call pre-emptive instabilities, which occur before they are expected on the basis of Plateau's laws.

Publicado em:
Soft Matter, 3 (2007)
47 – 57.

THE SHAPE OF SOAP FILMS AND PLATEAU BORDERS

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*Journal of Physics:
Condensed Matter* 19
(2007) 246106.

We have calculated the shapes of flat liquid films, and of the transition region to the associated Plateau borders (PBs), by integrating the Laplace equation with a position-dependent surface tension $\gamma(x)$, where $2x$ is the local film thickness. We discuss films in either zero or non-zero gravity, using standard $\gamma(x)$ potentials for the interaction between the two bounding surfaces. We have investigated the effects of the film flatness, liquid underpressure, and gravity on the shape of films and their PBs. Films may exhibit “humps” and/or “dips” associated with inflection points and minima of the film thickness. Finally, we propose an asymptotic analytical solution for the film width profile.

DEMIXING INSTABILITY IN COIL-ROD BLENDS UNDERGOING POLYCONDENSATION REACTIONS

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The authors extend their earlier work on the stability of a reacting binary polymer blend with respect to demixing [D.J. Read, *Macromolecules* 31, 899 (1998); P.I.C. Teixeira et al., *Macromolecules* 33, 387 (2000)] to the case where one of the polymers is rod-like and may order nematically. As before, the authors combine the random phase approximation for the free energy with a Markov chain model for the chemistry to obtain the spinodal as a function of the relevant degrees of reaction. These are then calculated by assuming a simple second-order chemical kinetics. Results are presented, for linear systems, which illustrate the effects of varying the proportion of coils and rods, their relative sizes, and the strength of the nematic interaction between the rods.

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Journal of Chemical Physics, 126 (2007) 074901.

LINE TENSION AND EXCESS ENERGY OF A WALL PLATEAU BORDER

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Physical Review E, 75
(2007) 011404.

We have calculated the equilibrium shape of the axially symmetric Plateau border (PB) along which a spherical bubble contacts a flat wall, by numerical integration of Laplace's equation. We found that the (spherical) film prolongation into the PB meets the wall at an internal angle $\phi \leq \pi/2$; the deviation $\Delta\phi$ equivalent to $\pi/2 - \phi$ is an increasing function of the liquid fraction and of the liquid-wall contact angle. For the equivalent dry bubble (*i.e.*, no PB) this deviation can be accounted for in terms of a negative line tension τ associated with the PB, and which can be determined from $\Delta\phi$. We have also calculated the (negative) PB excess energy ϵ , defined as the energy per unit length of the PB's liquid-gas and liquid-wall interfaces minus that of the film prolongation into the PB and of the dry wall. For $A^{1/2}/x(l) \leq 0.4$ (where A is the PB cross-sectional area and $x(l)$ is the radius of the extrapolated contact line), it was found that $\tau \propto \epsilon$. Finally, we derived a general relationship involving ϵ , τ and A which yields $\tau = \epsilon/2$ when $\tau \propto \epsilon$, *i.e.*, for not too large PBs; larger PBs have $\tau \propto \epsilon^{1/2}$.

INSTABILITIES IN TWO-DIMENSIONAL FLOWER AND CHAIN CLUSTERS OF BUBBLES

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We assess the stability of simple two-dimensional clusters of bubbles relative to small displacements of the vertices, at fixed bubble areas. The clusters analysed are: (1) flower clusters consisting of a central bubble of area λ surrounded by N shells each containing n bubbles of unit area, (2) periodic chain clusters consisting of N “parallel” rows of n bubbles of unit area and width w . The energy and bubble pressures of the symmetrical, unbuckled clusters are found analytically as a function of λ and w for given N and n . Both types of clusters studied show a single energy minimum at a critical λ_m or w_m . At the energy minimum for flower clusters, the pressure in the central bubble vanishes. The clusters show a symmetry-breaking buckling instability under compression at a critical λ_m or w_m . The corresponding critical energy E_b was determined with the Surface Evolver software. While for $N=1$ the conditions $\lambda_b=\lambda_m$, $w_b=w_m$ and $E_b = E_m$ hold, for $N > 1$ buckling requires further compression beyond the minimum, for which the energy increases with increasing compression (decreasing λ or w), and the excess pressure in the central bubble of the flower clusters becomes negative.

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*Colloids and Surfaces
A – Physicochemical
and Engineering
Aspects*, 309 (2007)
64-70.

ENERGY AND TENSION OF FILMS AND PLATEAU BORDERS IN A FOAM

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Publicado em:
Colloids and Surfaces
A – Physicochemical
and Engineering
Aspects, 309
 (2007) 3-6.

We discuss a number of problems relating to the energy and geometry of liquid foams in three dimensions. We use Plateau's concept of a skeletonised or ideal dry foam, consisting of geometrical surfaces, lines and points, which correspond, respectively, to the films, Plateau borders and nodes of the real foam, but including the contributions of all these elements to the total foam energy (and not just the film energy, as is usually done). In order to be able to write down all these contributions for a real foam, we conjecture that the same can be skeletonised by successively replacing the films by their mid-surfaces, the Plateau borders by the edges along which the mid-surfaces meet, and the nodes by the points where four edges are joined. We then relate the film energy γ and the film tension σ (energy per unit area), and define a Plateau border line tension τ (energy per unit length) and a node energy υ . The Plateau border line tension is negative and causes deviations from 120° of the angles between films, and from $\cos^{-1}(-1/3)$ of the angles between lines at nodes. We further define the excess energy ε of a Plateau border relative to the dry line. We illustrate our findings with calculations performed for a few simple systems – the double bubble, the lens bubble, and a bubble at a plate – for which skeletonisation is straightforward, and show that $\tau = \varepsilon/2$ when $\varepsilon \propto A^{1/2}$, with A the Plateau border cross-sectional area, *i.e.*, for not too high liquid fractions.

THE SPIN POLARISATION OF CrO_2 REVISITED

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Here, we use Andreev reflection spectroscopy to study the spin polarization of high quality CrO_2 films. We study the spin polarization as a function of growth temperature, resulting in grain size and electrical resistivity. In these films low temperature growth appears to be a necessary but not sufficient condition to guarantee the observation of high spin polarization, and this is only observed in conjunction with suppressed superconducting gap values and anomalously low interface properties. We suggest that this combination of observations is a manifestation of the long range spin triplet proximity effect.

Publicado em:

*Applied Physics
Letters*, 91 (2007)
172504 – 172507.

INFLUENCE OF GROWTH TEMPERATURE AND CARRIER FLUX ON THE STRUCTURE AND TRANSPORT PROPERTIES OF HIGHLY-ORIENTED CrO₂ ON Al₂O₃ (0001)

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Publicado em:
*Chemical Vapor
Deposition*, 13 (2007)
537 – 545.

In this work we report on the structure and magnetic and electrical transport properties of CrO₂ films deposited onto (0001) sapphire by atmospheric pressure (AP)CVD from a CrO₃ precursor. Films are grown within a broad range of deposition temperatures, from 320°C to 410°C, and oxygen carrier gas flow rates of 50–500 sccm, showing that it is viable to grow highly oriented a-axis CrO₂ films at temperatures as low as 330°C *i.e.*, 60–70°C lower than is reported in published data for the same chemical system. Depending on the experimental conditions, growth kinetic regimes dominated either by surface reaction or by mass-transport mechanisms are identified. The growth of a Cr₂O₃ interfacial layer as an intrinsic feature of the deposition process is studied and discussed. Films synthesized at 330°C keep the same high quality magnetic and transport properties as those deposited at higher temperatures.

ANISOTROPIC FERROMAGNETISM INDUCED IN RUTILE SINGLE CRYSTALS BY Co IMPLANTATION

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The magnetic and electrical properties of Co-implanted single crystalline TiO₂ rutile are presented. For fluences of the order of 10^{17} cm⁻² and implantation energy of 150keV the maximum atomic concentration of cobalt is 13 at% at a depth of 65nm from the surface. The as implanted single crystals exhibit superparamagnetic behaviour attributed to the formation of nanosized cobalt clusters. After annealing at 1073K an anisotropic ferromagnetic behaviour emerges with the easy magnetization axis lying in the (001) plane of rutile. The ferromagnetic behaviour is associated with oriented cobalt aggregates. Electrical conductivity of the implanted samples annealed in vacuum also exhibits anisotropic behaviour at low temperatures, but no magnetoresistive effects were detected.

Publicado em:

The European Physical Journal B, 55 (2007) 253-260.

EXPERIMENTAL RESULTS ON THE RHEOLOGICAL AND RHEO-OPTICAL BEHAVIOUR OF PET/LIQUID CRYSTALLINE POLYMER BLENDS

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Publicado em:

Journal of Applied Polymer Science, 107 (2007) 1280 – 1287.

The use of thermoplastic/liquid crystalline polymer (LCP) blends is recognized as a good strategy to reduce the viscosity and to improve the mechanical properties relatively to the pure thermoplastic. This improvement, however, is only noticeable if the LCP fibrillates, *in situ*, during processing, and the fibrils are kept in the solid state.

On this work we report the morphological, rheological and reo-optics study performed with two blends of polyethylenetereftalate (PET) with a liquid crystalline polymer, Rodrun LC3000 (10 and 25wt% LCP content) and we show that, specially the obtained *droplet shape relaxation time* (the time the deformed droplet takes to regain its spherical form after cessation of flow) allows for the explanation of the morphological observations. In fact the *droplet shape relaxation time* is higher for the blend with higher LCP content, for the higher experimentally accessible shear rates, and is still increasing at the highest shear rate, which explain the fibrils of the LCP dispersed phase observed in this blend, while in the case of the lower LCP content blend the *droplet shape relaxation time* reaches a low value plateau for higher shear rates, which explains the absence of fibrillation in this blend.

A NEW BRIDGE BETWEEN LEPTONIC CP VIOLATION AND LEPTOGENESIS

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Flavour effects due to lepton interactions in the early Universe may have played an important role in the generation of the cosmological baryon asymmetry through leptogenesis. If the only source of high-energy CP violation comes from the left-handed leptonic sector, then it is possible to establish a bridge between flavoured leptogenesis and low-energy leptonic CP violation. We explore this connection taking into account our present knowledge about low-energy neutrino parameters and the matter-antimatter asymmetry observed in the Universe. In this framework, we find that leptogenesis favours a hierarchical light neutrino mass spectrum, while for quasi-degenerate and inverted hierarchical neutrino masses there is a very narrow allowed window. The absolute neutrino mass scale turns out to be $m \leq 0.1$ eV.

Publicado em:

Physics Letters B,
645 (2007) 432 - 436.

NATURAL GAUGE AND GRAVITATIONAL COUPLING UNIFICATION AND THE SUPERPARTNER MASSES

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The possibility to achieve unification at the string scale in the context of the simplest supersymmetric grand unified theory is investigated. We find conservative upper bounds on the superpartner masses consistent with the unification of gauge and gravitational couplings, TeV and GeV, for the superparticles with spin one-half and zero, respectively. These bounds hint towards the possibility that this supersymmetric scenario could be tested at future colliders, and in particular, at the forthcoming LHC.

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Physics Letters B, 648
(2007) 60 - 63.

NEUTRAL MINIMA IN TWO-HIGGS DOUBLET MODELS

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We study the neutral minima of two-Higgs doublet models, showing that these potentials can have at least two such minima with different depths. We analyse the phenomenology of these minima for the several types of two-Higgs doublet potentials, where CP is explicitly broken, spontaneously broken or preserved. We discover that it is possible to have a neutral minimum in these potentials where the masses of the known particles have their standard values, with another deeper minimum where those same particles acquire different masses.

Publicado em:

Physics Letters B, 652
(2007) 181 - 193.

LEPTON FLAVOUR VIOLATING PROCESSES AT THE INTERNATIONAL LINEAR COLLIDER

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We study the effects of dimension six effective operators on the flavour violating production and decay of leptons at the International Linear Collider. Analytic expressions for the cross sections, decay widths and asymmetries of all flavour changing processes will be presented, as well as an analysis of the feasibility of their observation at the ILC.

Publicado em:

Physical Review D, 75
(2007) 055015 -
055031.

CRUSTAL SEISMIC VELOCITY STRUCTURE NEAR FAIAL AND PICO ISLANDS (AZORES), FROM LOCAL EARTHQUAKE TOMOGRAPHY

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The Azores archipelago (Portugal) is located on an oceanic plateau, in a geodynamic environment prone to intense seismic and volcanic activity. In order to investigate the crustal structure in this region, we have conducted a local earthquake tomography study in the area of the islands of Faial, Pico and S. Jorge using data recorded in July 1998. The July 9th 1998 earthquake, near Faial Island, triggered an aftershock sequence of thousands of events that lasted for several months and were recorded by a total of 14 stations located on the three islands surrounding the epicentral area.

In the upper crustal layers, consistency is seen between the tomographic results and the islands' surface volcanic units. Beneath the Faial central volcano a low V_p (<6.0 km/s) anomaly roughly located at 3-7 km depth, suggests a connection to the plumbing system, possibly the presence of a magma chamber. In NE Faial, a high V_p (>6.3 km/s) body was found located at mid-lower crust, most likely an intrusion of gabbroic composition, that is bordered by the registered seismic activity; its shape suggesting a tectonic controlled mechanism. The relocated hypocenters, together with the overall analysis of the Tomographic model, suggest a tectonic segmentation of Faial Island. The crustal thickness under the islands volcanic buildings of the Faial-Pico area was estimated at around 14 km.

Publicado em:

Tectonophysics, 445
(3-4) (2007) 301-317.

THE 9th OF JULY 1998 FAIAL ISLAND (AZORES, NORTH ATLANTIC) SEISMIC SEQUENCE

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Publicado em:

Journal of Seismology,
11(3) (2007) 275-298.

The Faial earthquake (ML 5.8) that occurred on the 9th of July 1998, in the Azores region (north Atlantic), caused 9 casualties and severe destruction affecting more than 5000 people. The main shock located at sea, 10km NE of the Faial Island, triggered a seismic sequence that lasted for several weeks and was characterized by an unusual high p-value of 1.40 for the modified Omori law.

In this work we present the results of a joint inversion of hypocenters and 1D velocity model performed on the data collected by the permanent network complemented with a temporary network installed shortly after the main event.

The 1D velocity model shows a heterogeneous upper crust, testified by the observed differences in site effects at the stations, while the middle crust from ~2.5 to 8km depth is quite homogeneous. The Moho is located at about 12-13km depth and the Vp/Vs ratio is found to be around 1.78. The events at depth are mainly concentrated in the middle-lower crust (8-12km) while their spatial distribution shows a main cluster, visible after relocation, trending SSE. This direction of elongation is consistent with one of the fault planes (N151°E) of the CMT solution for the main shock. The same plane is the preferred main shock fault plane inferred after a Coulomb Failure Function analysis on the aftershock distribution. The main event relocation points to a shallow source.

The aftershocks pattern shows that several fault systems were reactivated by the main shock. Besides the two main tectonic directions, trending WNW-ESE and NNW-SSE, that are also observed in the tectonics of Faial, Pico and S. Jorge, there is also evidence of a new tectonic direction trending WSW-ENE.

THE ELASTIC BOUNCES OF A SPHERE BETWEEN TWO PARALLEL WALLS

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The kinematics of a sphere of radius R and mass m bouncing elastically in a horizontal channel is studied in detail. Explicit expressions for the position and linear and angular velocities of the sphere at any collision are obtained. It is shown that if the moment of inertia $I = \frac{1}{2}mR^2$ is such that $(1-\epsilon)/(1+\epsilon) = \cos^2 \alpha/k$ with k an integer and $k \geq 4$, the motion is periodic, with repetition after k collisions for k even, and after $2k$ collisions for k odd. The motion of a homogeneous sphere (which is not periodic) is analyzed by investigating the mean properties of its velocities and positions. The analogy between this motion and that of a periodic oscillator is discussed.

Publicado em:

The American Journal of Physics, 75 (2007) 690 – 695.

ON THE RELATION BETWEEN ANGULAR MOMENTUM AND ANGULAR VELOCITY

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Publicado em:
*American Journal of
Physics, 75 (2007)
53-55.*

Mechanics students usually face some challenges when they learn about rotation of a rigid body. This difficulty is rooted in the relation between angular momentum and angular velocity, both because these vectors are not parallel and because one is in general forced to utilize a rotating frame of reference (or else, deal with a time dependent inertia tensor). Here we discuss a series of simple exercises which introduce both problems.

RECENT IMPROVEMENTS IN THE BROADBAND SEISMIC NETWORKS IN PORTUGAL

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Portugal, in spite of the significant earthquake region, (e.g.: Borges et al., 2001) has been operating a limited number of broadband digital seismic instruments. The older BB seismic station in a systematic and continuous operation on the country is MTE, belonging to GEOFON and locally supported by IM, which is working since 1997. To efficiently carry out the task of develop the Broadband Portuguese seismic network, there is a collaboration between some national institutions, such as Institute of Meteorology (IM), Geophysics Center of Évora University (CGE/UE), Geophysics Center of University of Lisbon (CGUL/IGIDL) and Instituto Superior Técnico (IST), with governmental support from the National Science and Technology Foundation (Rede Nacional de Geofísica, RNG). From this collaboration we expect shortly to assist the emergence of a high quality infrastructure, significant to real-time monitoring the earthquake activity for use by governmental authorities, and of paramount importance to scientific research. The installation of this network is to be carried out in narrow connection with international institutions as GEOFON, EMSC, ROA, ORFEUS, with who we saw to establish collaborations. Data from some stations are already being exported to international data centers, such as DMC and ORFEUS, and will be used for an upcoming prototype of an Early Warning Tsunami System to be developed for Cadiz Gulf coastal area and southwestern coasts of Portugal mainland, within the framework of the NEAREST project. While the broadband network is developed they elapse investigation projects that request short period data. Of these projects we highlight the Seismic Tomography of the Continental Lithosphere of Algarve (Portugal) that involve the installation of a Portable seismic network consisting of 30 short period stations, including a subnet of 7 telemetry stations, in operation since January 2006.

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THE SHAPE OF SOAP FILMS AND PLATEAU BORDERS

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Matter Conference",
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2007 (comunicação
em poster).*

We have calculated the shapes of flat liquid films, and of the transition region to the associated Plateau borders (PBs), by integrating the Laplace equation with a position-dependent surface tension $\gamma(x)$, where $2x$ is the local film thickness. We discuss films in either zero or non-zero gravity, using standard $\gamma(x)$ potentials for the interaction between the two bounding surfaces. We have investigated the effects of the film flatness, liquid underpressure, and gravity on the shape of films and their PBs. Films may exhibit "humps" and/or "dips" associated with inflection points and minima of the film thickness. Finally, we propose an asymptotic analytical solution for the film width profile.

THE PHASE BEHAVIOUR OF A MODEL TETRAPODE – A THEORETICAL ANALYSIS

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The archetypal liquid crystal forming mesogen is a rigid rod or disc. Recently, however, it has been shown that flexible molecules also exhibit liquid crystalline phases – tetrapodes are a good example of these [1,2]. The molecules are able to exist in several stable conformations and, by preferentially selecting certain geometries, the molecules can advantageously pack into ordered mesoscopic phases. In other words, conformational disorder is sacrificed in order to achieve better packing.

Previous theoretical studies on such systems have been presented [3], but in order to capture the essential physics of the process, we present here a stripped-down model which permits a clear, detailed analysis and which also exhibits rich phase behaviour.

In our model a particle can exist in two states, corresponding to a prolate and an oblate spheroid. The energies of these two states differ by a prescribed amount and the two conformers are in chemical equilibrium. The interactions between the particles are described by the Gaussian Overlap Model [4] and we analyse the phase behaviour using a second virial (Onsager) approach, which, among other things, has been successfully used to understand the phase behaviour of binary mixtures of plate-like and rod-like particles [5].

Rod d/plate mixtures have been predicted to show complex phase behaviour. Depending on conditions one may find stable biaxial nematic phases and N⁺-N⁻ co-existence. In our model the rods and plates are inter-convertible, and the position of equilibrium is affected by the choice of energy difference between the states (as well as by their aspect ratios). We present a thorough analysis of the phase behaviour of our system as a function of this energy parameter and report on the stability of the biaxial phase.

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Livro de resumos da "9th European Conference on Liquid Crystals", ECLC2007, Lisboa, Portugal, 2007 (comunicação em poster).

FOAM-LIKE BEHAVIOUR OF LAMELLAR IONIC LIQUID CRYSTALS

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N-alkylimidazolium salts have been shown to order into either columnar and lamellar mesophases [1]. This liquid crystalline behaviour can be induced at room temperature by shear [2]. Sheared films of the

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R= n-alkil

lamellar phase of these compounds observed between crossed polars exhibit a morphology that is typical of (wet) liquid foams: they divide into dark domains separated by brighter (birefringent) walls which are approximately arcs of circle and meet in “Plateau borders” with three or more sides. Where walls meet three at a time, they do so at approximately 120° angles. These patterns coarsen with time, both T₁ and T₂ processes having been observed, as in foams. The time evolution of domains is also consistent with von Neumann’s law [3]: domains with fewer than 6 sides shrink and disappear, whereas those with 6 or more sides either remain unchanged or increase in area. (see figure 4). We conjecture that the bright walls are regions of high concentration of defects produced by shear, and that the system is dominated by the interfacial tension between these walls and the uniform domains.



Figure. 1

DISORDER AND THE SPIN POLARISATION OF CrO₂

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CrO₂ has attracted a great deal of interest because it has a high degree of spin polarization as measured by point contact Andreev reflection (PCAR) spectroscopy. Frequently those Andreev spectra that show very high P ($\geq 95\%$) also show a very low interface barrier “Z” [1,2], with reduced P values at higher Z being attributed to spin flip scattering from an interfacial layer. Here we study a selection of CrO₂ films using PCAR and anomalous Hall measurements. The films chosen have a wide range of residual resistivity ratios, and are grown by a low temperature chemical vapor deposition method [4]. As shown in the figure below, there is a clear correlation between high P and suppressed gap parameter as well as the previously observed remarkably low Z. Interestingly this combination of observations may relate to the claim that the long range spin triplet proximity effect can exist in this material [5]. Surprisingly we find that the films which show these effects are those with smaller grain size, increased surface roughness and higher values of low temperature resistivity (most likely due to the increased grain boundary contribution). The anomalous Hall measurements also show systematic trends with increased disorder and unlike previous reports [3] we find that the carriers are hole-like at all temperature in these films with hole mobility decreasing with increasing disorder.

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Spintronic Materials
and Technology”,
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poster).*

INFLUENCE OF NANOSIZED Cr_2O_3 INTERFACIAL LAYERS ON THE TRANSPORT AND MAGNETIC PROPERTIES OF CVD- CrO_2 /SAPPHIRE

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The ferromagnetic half-metallic nature of chromium dioxide (CrO_2) makes this compound one of the most attractive thin films material for potential use in spintronic devices. This work reports on the structure and magnetic and transport properties of CrO_2 films deposited onto (0001) Al_2O_3 by atmospheric pressure CVD from CrO_3 precursor. Films were grown within broad ranges for the deposition temperature, from 320°C to 410°C, and oxygen carrier gas flow rates, 50 – 500 sccm. We will show that it is viable to grow highly oriented (100) CrO_2 films at temperatures as low as 330°C, *i.e.* 60 – 70°C lower than in published data for the same chemical system.

The growth of a Cr_2O_3 layer with variable thickness, $d(\text{Cr}_2\text{O}_3)$, in the nanometer range, at the CrO_2 /substrate interface, was evidenced by the characterization methods and may be considered as an intrinsic feature of the CrO_2 synthesis process onto sapphire substrates. For high growth temperatures and short deposition times, the CrO_2 and Cr_2O_3 layers have similar thickness of a few decades of nm and we have observed a detrimental effect on the saturation magnetization and transport measurements of the stacked layers. As the deposition time increases, the Cr_2O_3 layer decreases to <20 nm, while total film thickness increases. A possible interpretation for this feature will be given based on a phase transformation, $\text{Cr}_2\text{O}_3 \rightarrow \text{CrO}_2$, induced by the relaxation of the stresses developed during film growth. As the $d(\text{Cr}_2\text{O}_3)/d(\text{CrO}_2)$ ratio remains under ca. 5%, a saturation magnetization value close to the bulk was measured at room temperature, and the dependence of the resistivity curve on temperature is in agreement with other data from literature.

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“European Materials
Research Society
Spring Meeting”,
E-MRS 2007,
Symposium H,
Strasbourg, France
(comunicação oral).

A NEW APPROACH TO SYNTHESIZE NANOCRYSTALLINE Co-DOPED TiO₂ THIN FILMS AT LOW TEMPERATURE

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Diluted magnetic semiconductors (DMS) exhibiting ferromagnetic behaviour above room temperature are key materials for the emerging new field of spintronics. Following theoretical predictions that doping of semiconductor oxide hosts with transition metals might introduce ferromagnetic ordering, several recent DMS have been studied. Among them, Co-doped anatase TiO₂ exhibit the highest Curie temperature (up to at least 500 K) and the highest saturation and remanent magnetization of any recently discovered oxide semiconductor. Such films have been grown using a wide variety of deposition methods, usually requiring deposition temperatures higher than 500°C, which could preclude interface quality and/or exclude the use of thermal sensitive substrates. Therefore, there is a continuous search for deposition techniques that allow the synthesis of Co-doped TiO₂ thin films at lower temperatures.

In this work we report on Co-doped TiO₂ thin films onto Si(100) and Al₂O₃ (0001) substrates, using dip- and spin-coating techniques via aqueous/organic suspensions at T < 200°C. The films precursor nanopowders were obtained using a novel and easy method based on a hydrothermal process via precipitation of TiCl₃.

Both Co-doped TiO₂ nanopowders and films were characterized by X-ray diffraction (XRD), electronic microscopy (SEM and TEM) and UV/Vis spectrophotometry. It will be discuss the influence of some experimental parameters, notably the Co-doping concentration, on the film properties.

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Livro de resumos do "European Materials Research Society Spring Meeting", Symposium H, Strasbourg, France (comunicação em poster).

LEPTON FLAVOUR VIOLATION AT THE ILC

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We explore the possibility of detecting lepton flavour violation, now a well established experimental fact, at the International Linear Collider. Using a model independent approach we conclude that, given all experimental constraints available, there is still room to detect lepton flavour violation at the ILC.

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Livro de resumos da conferência "XXVII Physics in Collision", Annecy, France, 2007 (apresentação em poster).

STRUCTURAL AND MICROANALYTICAL STUDIES OF CrO₂ THIN FILMS ON c-SAPPHIRE BY HIGH RESOLUTION ELECTRON MICROSCOPY METHODS

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Chromium dioxide (CrO₂) has been extensively used in the magnetic recording industry. However, it is its ferromagnetic half-metallic nature that has more recently attracted much attention, primarily for the development of spintronic devices. CrO₂ is the only stoichiometric binary oxide theoretically predicted to be fully spin polarized at the Fermi level. It presents a Curie temperature of ~ 396K, *i.e.* well above room temperature, and a magnetic moment of 2 μ_B/formula unit. These properties make chromium dioxide a promising material to be used in magnetoresistive structures. It should also be noted that many of the proposed devices demand carefully controlled growth of interfaces that can be achieved by preparing thin films at sufficiently low temperatures to ensure interface quality and avoid substrate damage.

Here we report on high resolution electron microscopy structural and analytical studies of CrO₂ films deposited onto (0001) sapphire by atmospheric pressure CVD from CrO₃ precursor. Films were grown within a broad range of deposition temperatures from 320°C to 410°C, and oxygen carrier gas flow rates of 50 – 500sccm.

Cross-sectional specimens for TEM were prepared by mechanical grinding, dimpling and argon ion-milling of the samples in a liquid-nitrogen-cooled holder with an acceleration voltage of 5kV and an incidence angle of 8°. Analytical TEM and HREM studies were carried out using a Philips Tecnai 20F FEG microscope operating at 200kV, equipped with an Energy Dispersive X-Ray (EDX) analysis system and a scanning transmission electron microscopy modulus (STEM) with a high angle annular detector (HAAD) for Z-contrast imaging and composition mapping. Electron diffraction pattern (EDP) and simulations using Fast Fourier transform (FFT) of the HREM images were used to analyze the crystal structure.

TEM results indicate that the deposited layers are composed of both Cr₂O₃ with corundum crystal structure and CrO₂ with rutile crystal structure. After selected area diffraction pattern and Fast Fourier transform simulations the orientation relationship was determined: [01-10] Al₂O₃ || [01-10] Cr₂O₃ || [001] CrO₂ and [1-210] Al₂O₃ || [1-210]

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Microscopy and
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$\text{Cr}_2\text{O}_3 \parallel [010] \text{CrO}_2$. At the interface, Cr_2O_3 with corundum structure parallel to the Al_2O_3 substrate was observed, the interface appear sharp and free of defects except for those samples deposited at of 360°C where a three-dimensional growth of the Cr_2O_3 bottom layer was observed.

A NEW CHEMICAL ROUTE TO SYNTHESISE TM-DOPED (TM = Co, Fe) TiO₂ NANOPARTICLES

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Diluted magnetic semiconductors (DMS) exhibiting ferromagnetic behaviour above room temperature are considered key materials for the development of spintronic devices. Among them, TM-doped (TM = Co, Fe) TiO₂ based oxides are considered very promising materials to achieve such goals.

In this work we report a new and swift chemical route to synthesise nanoparticles of such oxides. The synthesis of Ti_{1-x}TM_xO₂ (0 ≤ x ≤ 0.10) anatase phase nanocrystallites was achieved via precipitation of acid solutions of TiCl₃ and TM chlorides with ammonia followed by thermal treatment in autoclave with different suspension media. The Ti_{1-x}TM_xO₂ nanoparticles can be easily stored in suspensions and straightforwardly retrieved by centrifugation whenever necessary. Using such facility, thin films of Ti_{1-x}TM_xO₂ onto Si (100) substrates were prepared by dip- and spin-coating technique.

Both TM-doped TiO₂ nanopowders and films were characterised by X-ray diffraction (XRD), electronic microscopy (TEM and SEM), energy dispersive spectroscopy (EDS), atomic force microscopy (AFM) and absorption spectroscopy.

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Livro de resumos do "European Materials Research Society Fall Meeting", Symposium A, Warsaw, Poland (comunicação oral).

STRUCTURAL CHARACTERIZATION OF NANOSTRUCTURES BASED ON CVD CHROMIUM DIOXIDE

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Chromium dioxide (CrO_2) is one of the most attractive ferromagnetic compounds being investigated for potential use in spintronic devices. Many of the proposed devices demand carefully controlled growth of interfaces that can be achieved by preparing thin films at sufficiently low temperatures to ensure interface quality and avoid substrate damage.

In this work, we report on the structural characterization of thin films grown onto Al_2O_3 (0001) by atmospheric pressure chemical vapour deposition (APCVD) from CrO_3 precursor. Phase composition, crystalline quality and surface morphology of the films were studied as a function of the oxygen carrier gas flux and growth temperature, from 410°C down to 320°C . We will show that structural properties are very responsive to the processing parameters. X-ray diffraction results demonstrate the synthesis of highly oriented a-axis CrO_2 films at temperatures as low as 330°C *i.e.* 70°C lower than for previously published data. The existence of a Cr_2O_3 antiferromagnetic interlayer, a few nanometres thick, between the CrO_2 and the sapphire substrate is discussed.

The microstructure and surface roughness of the as-grown layers were studied by atomic force microscopy (AFM) and were shown to depend mainly on film thickness.

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on Structural
characterization of
nanostructures",
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Universidade de
Aveiro, Portugal, 2007
(comunicação oral).

ANCHORING TRANSITION OF NEMATIC LIQUID CRYSTALS IN PATTERNED CELLS. EFFECT OF CONFINEMENT AND ELECTRIC FIELD

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We generalize the study of the geometrically-controlled twist transition in nematic cells [1] by taking into account the effect of electric field. We have developed a Newton branch following method based on implicit relaxation timestep. This method provides a direct solution of the Euler-Lagrange equations satisfied by the extrema of the free energy functional. Standard minimization methods are not applicable to this problem as the functional has no minima in the presence of the electric field. In order to take into account the planar degenerate weak anchoring at the surface of the cell, we introduce a generalization of the Nobili-Durand substrate potential which is only valid for homeotropic anchoring.

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INTERACTIONS BETWEEN CIRCULAR INCLUSIONS IN SMECTIC-C FILMS WITH PLANAR ANCHORING

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We investigate analytically the interaction between circular inclusions in smectic-c films with planar anchoring. We present a rigorous solution for an isolated circular colloid with planar anchoring and use it to calculate the interaction between two circular colloids, approximately. At large separations the interaction is quadrupolar and we show that at short range two different regimes may be observed. For weak anchoring, the interaction is always attractive in some directions, which may lead to particle contact or coalescence. However, for strong anchoring, the interaction exhibits a well defined minimum, for colloids at a particular separation and given relative orientation. The equilibrium configuration was found to depend on the anchoring strength.

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Crystals”, Lisboa,
Portugal (comunicação
em poster).*

COMPLETE WETTING TRANSITIONS OF NEMATIC LIQUID CRYSTALS ON A STRUCTURED SUBSTRATE

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It is known that the wetting behaviour of a fluid is deeply altered in the presence of rough or structured substrates. We will first review some simple considerations about isotropic fluids and rough substrates, and then we will generalize Wenzel's law, which assigns an effective contact angle for a droplet on a rough substrate, when the wetting layer has an ordered phase, like a nematic. We estimate the conditions for which the wetting behaviour of an ordered fluid can be qualitatively different from the one usually found in a simple fluid. To particularize our general considerations, we will use the Landau-de Gennes mean field approach to investigate theoretically and numerically the complete wetting transition between a nematic liquid crystal and a periodic triangular structured substrate.

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MULTIFRACTAL ANALYSIS OF DEPOSITS OF DIPOLAR PARTICLES

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Computer simulations are used to generate two-dimensional diffusion-limited deposits of dipoles. These deposits are used to obtain the growth probability measure through Monte Carlo techniques. It is found that the distribution of growth probabilities obeys multifractal scaling, *i.e.*, it can be analyzed in terms of its $f(a)$ multifractal spectrum. For low dipolar strengths, the $f(a)$ spectrum is similar to that of diffusion-limited aggregation. Our results suggest that for increasing dipolar strength both the minimal local growth exponent a_{\min} and the information dimension D_1 decrease, while the fractal dimension remains the same.

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poster).*

COHERENCE THRESHOLD IN EVOLUTIONARY LANGUAGE GAMES

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A simple model of language evolution proposed by Komarova, Niyogi, and Nowak is characterized by a payoff in communicative function and by an error in learning that measure the accuracy in language acquisition. The time scale for language change is generational, and the model's equations in the mean-field approximation are a particular case of the replicator-mutator equations of evolutionary dynamics. In well-mixed populations, this model exhibits a critical coherence threshold; *i.e.*, a minimal accuracy in the learning process is required to maintain linguistic coherence. In this work, we analyze in detail the effects of different fitness-based dynamics driving linguistic coherence and of the network of interactions on the nature of the coherence threshold by performing numerical simulations and theoretical analyses of three different models of language change in finite populations with two types of structure: fully connected networks and regular random graphs. We find that although the threshold of the original replicator-mutator evolutionary model is robust with respect to the structure of the network of contacts, the coherence threshold of related fitness-driven models may be strongly affected by this feature.

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SUPERCONDUCTIVITY IN THE NEW $Y_3Os_8B_6$ BORIDE

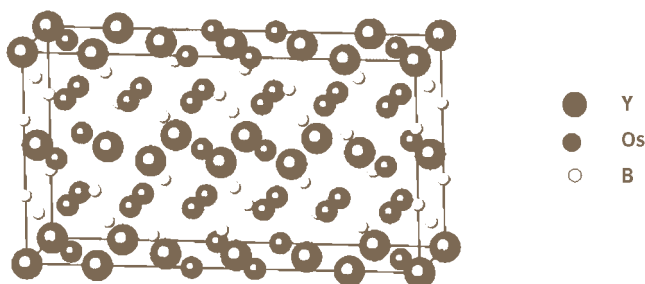
Lopes, E.B.¹; Sologub, O.L.^{1,2}; Casaca, A.^{1,3};
Havela, L.⁴; Sebek, J.⁵; Santava, E.⁵; Janu, Z.⁵;
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A recently discovered $Y_3Os_8B_6$ ternary boride was prepared by arc melting. This compound crystallizes in the $Ca_3Rh_8B_6$ type-structure, which is closely related with the $CeCo_3B_2$ -type. Ac-susceptibility, magnetization, electrical resistivity and specific heat measurements show that $Y_3Os_8B_6$ is a new type II superconductor with a transition temperature, T_C , of 5.8(3) K and a maximum upper critical field, $B_{c2}(0)$, of ~2 T. $Y_3Os_8B_6$ is the first representative of a possible new family of superconducting borides. The structure and properties of this compound are discussed in relation to other ternary superconducting borides.

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Actinides", Sesimbra,
Portugal, 2007
(comunicação oral).



HIGHLY SPIN POLARISED CHROMIUM DIOXIDE FILMS GROWN ON SAPPHIRE BY ATMOSPHERIC PRESSURE CVD

Sousa, P.M.¹; Dias, S.A.¹; Silvestre, A.J.²;
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Chromium dioxide (CrO₂) is one of the most attractive ferromagnetic compounds being investigated for potential use in spintronic devices. Many of the proposed devices demand carefully controlled growth of interfaces that can be achieved by preparing thin films at sufficiently low temperatures to ensure interface quality and avoid substrate damage.

In this work, we report on the structural characterization of thin films grown onto Al₂O₃ (0001) by atmospheric pressure chemical vapour deposition (APCVD) from CrO₃ precursor. Phase composition, crystalline quality and surface morphology of the films were studied as a function of the oxygen carrier gas flux and growth temperature, from 410°C down to 320°C. We will show that structural properties are very responsive to the processing parameters. X-ray diffraction results demonstrate the synthesis of highly oriented a-axis CrO₂ films at temperatures as low as 330°C *i.e.* 70°C lower than for previously published data. The existence of a Cr₂O₃ antiferromagnetic interlayer, a few nanometres thick, between the CrO₂ and the sapphire substrate is discussed.

The microstructure and surface roughness of the as-grown layers were studied by atomic force microscopy (AFM) and were shown to depend mainly on film thickness.

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Livro de resumos da conferência "MATERIAIS 2007 – Global Materials for the XXI Century: Challenges to Academia and Industry, 4th Int. Materials Symposium", Universidade do Porto, Portugal, (comunicação em poster).

SYNTHESIS OF Co-DOPED TiO₂ THIN FILMS AT ROOM TEMPERATURE

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Key materials for the emerging new field of spintronics are diluted magnetic semiconductors (DMS) exhibiting ferromagnetic behaviour above room temperature. Following theoretical predictions that doping of semiconductor oxide hosts with transition metals might introduce ferromagnetic ordering, several recent DMS have been studied. Among them, Co-doped anatase TiO₂ exhibit the highest T_c (up to at least 500K) and the highest saturation and remanent magnetization of any recently discovered oxide semiconductors. Such films have been grown using a wide variety of deposition methods, usually requiring deposition temperatures higher than 500°C, which could preclude interface quality and/or exclude the use of thermal sensitive substrates. Therefore, there is a continuous search for deposition techniques that allow the synthesis of Co-doped TiO₂ thin films at lower temperatures.

In this work we report on the deposition of Co-doped TiO₂ thin films onto Si (100) substrates. The films were prepared from Ti_{1-x}Co_xO₂ nanopowders suspensions by dip-coating technique followed by post-annealing at T = 200°C in vacuum. Both nanopowders and films were analyzed by X-ray diffraction (XRD) and transmission electron microscopy (TEM), electron diffraction and energy dispersive X-ray spectroscopy (EDS).

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A CRISE SÍSMICA DO FAIAL DE JULHO DE 1998: ESTRUTURA CRUSTAL E CARACTERÍSTICAS ESPÁCIO-TEMPORAIS

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A monitorização instrumental reforçada da crise sísmica do Faial de Julho de 1998 permitiu uma cobertura adequada para um estudo aprofundado da características da sismicidade (taxas de ocorrência, estruturas sismogénicas principais, mecanismos de geração) e da estrutura crustal da região (tipo de litosfera, modelação 1-D e 3-D, estado de tensão crustal e o nível de fissuração existente).

A inversão 1-D e 3-D indica que a crosta sob as ilhas do Faial e Pico possui uma estrutura superficial heterogénea e uma crosta média-inferior bastante homogénea, com a Moho a 12-13km. Este aumento de espessura em relação a uma crosta oceânica “típica” é devida a um espessamento da camada 3. Na área de maior actividade sísmica, detectou-se a um corpo de elevado V_p , interpretado como a uma intrusão cristalina de rochas máficas (Gabros) e ultra-máficas, sendo também clara a assinatura das câmaras magmáticas sob os principais edifícios vulcânicos do Faial e Pico. Existe a indicação de um acidente tectónico em profundidade paralelo à cadeia Faial-Pico, que limita a propagação da sismicidade para o canal de S. Jorge, sendo sugerida a segmentação da ilha do Faial em 2 sectores.

Foi detectada anisotropia sísmica sob as estações compatível com o modelo EDA, com correlação entre o índice de fracturação e o posicionamento de cada estação. A orientação estimada para a direcção de compressão horizontal máxima, indica um complexo padrão nas trajectórias da tensão com rotação da direcção NW-SE para SW-NE no sector oriental da ilha do Faial prolongando-se para o mar.

A distribuição da sismicidade indica que das estruturas tectónicas principais existentes, a mais activa corresponde à de orientação NNW-SSE com desligamento esquerdo dominante, existindo uma direcção secundária WSW-ENE de desligamento direito. As estruturas NW-SE desempenham um papel essencialmente confinante da sismicidade.

Publicado em:

Livro de resumos do “5.º Simpósio de Meteorologia e Geofísica da APMG”, APMG2007, Peniche, Portugal (comunicação oral).

UTILIZAÇÃO DE TÉCNICAS TAXONÓMICAS NA ANÁLISE DE SISMOS: O CASO DA CRISE SÍSMICA DO FAIAL DE JULHO DE 1998

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Na modelação da actividade sísmica é geralmente assumido que esta possui um comportamento espacio-temporal passível de ser descrito por uma distribuição de Poisson; contudo, a análise das distribuições de réplicas e/ou percursos associadas a grandes eventos mostram frequentemente uma grande correlação entre estes eventos, com tendência para o agrupamento espacial e temporal dos focos sísmicos, estando ainda associados a mecanismos focais e formas de onda registadas semelhantes.

Essa similaridade implica: i) para a função-fonte, os eventos possuírem mecanismos focais do mesmo tipo e magnitudes da mesma ordem; ii) que percursos de propagação similares necessitam de aglomeração espacial dos eventos, de escala inferior às dimensões das heterogeneidades próximas da fonte e dos comprimentos de onda observados.

O cumprimento desta condições conduzem a agrupamentos de sismos, cuja distinção se baseia no grau de semelhança exibido pelos sinais gerados por cada evento registados numa rede sismológica. O grau de semelhança existente entre formas de onda registadas (sismogramas) pode então ser utilizado na obtenção de uma estimativa precisa da localização relativa dos eventos pertencentes a um dado conjunto, da sua distinção e associação a estruturas geológicas específicas ou do correspondente mecanismo gerador cujo constrangimento será mais rigoroso.

Tais técnicas permitem também a correcção das observações instrumentais, como o acerto de chegadas de fases sísmicas similares, correcção de polaridades em fases pouco energéticas ou a correcção das orientações de sensores analógicos.

No caso da crise sísmica do Faial, estas técnicas permitiram a distinção entre as várias zonas sismogénicas, nomeadamente em termos da sua definição precisa e no cálculo de mecanismos focais compostos, associados às várias “famílias” de sismos analisadas e classificadas.

Publicado em:

Livro de resumos do “5.º Simpósio de Meteorologia e Geofísica da APMG”, APMG2007, Peniche, Portugal (comunicação oral).

SHALLOW CRUSTAL STRUCTURE BENEATH THE AZORES FROM AMBIENT SEISMIC NOISE CROSS-CORRELATION

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The Azores Islands mark the surface expression of a large submarine plateau roughly of triangular shape extending through African, Eurasian and American plates. Due to a complex tectonic environment, the Azores crust, exhibits important deep and lateral variations in both structure and composition. The goal of this study is to contribute for a better knowledge of the Azores shallow crust, using ambient seismic noise.

A preliminary analysis of the noise cross-correlation between seismic records obtained in a temporary VBB network, from October 2000 to September 2002, revealed that the source of the long period seismic noise is mainly induced by oceanic storms and it is located in the South hemisphere during summer (South Indian and South Pacific) and on North hemisphere (North Atlantic) during winter. The study of the cross-correlogram, at different frequency bandwidths, has shown that we can extract the Green's function between 5 and 30 seconds. We present here the preliminary group velocity dispersion curves obtained between different station pairs across the Azores archipelago.

Publicado em:

*Livro de resumos do
"5.º Simpósio de
Meteorologia e
Geofísica da APMG",
APMG2007, Peniche,
Portugal (comunicação
oral).*

SHALLOW CRUSTAL STRUCTURE OF PONTA DELGADA REGION

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Seismic noise analysis has been applied to a few sites in Ponta Delgada town, in order to evaluate the shallow shear-wave velocity profiles, which are essential for estimation of seismic site response.

It has been demonstrated that the cross correlation of seismic noise between a pair of stations contains, at least partially, the Green function between the two stations [Shapiro and Campillo, 2004; Sabra et al., 2005]. This Green function can be used to extract the group velocity between the stations pair and, after that, inverted to retrieve shear wave velocity profiles for the shallow structure.

The cross-correlation between each stations pair has been computed at different frequency bands to better comprehend the noise origin. The analysis of the correlograms, obtained without filtering, only reflect the presence of a low frequency noise, probably induced by the sea. Between 0.8 and 2Hz we have been able to retrieve a good Green function. At a frequency band of 2 – 4Hz the noise reveals, mainly, human activity. Computation of the Rayleigh wave group velocities is now underway.

Publicado em:

*Livro de resumos do
"5.º Simpósio de
Meteorologia e
Geofísica da APMG",
APMG2007, Peniche,
Portugal (comunicação
oral).*

CHARACTERIZATION OF THE ANISOTROPY IN THE MANTLE BENEATH MANTEIGAS FROM SPLITTING OF SKS WAVES

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The Variscan Iberian Massif covers a large area of central and western Iberia. A better characterization of mantle anisotropy is important, not only at this part of the Iberian Peninsula, as well to provide new insight in mantle anisotropy below this class of orogens. The Geofon VBB seismic station MTE (Manteigas), located in the western part of the Peninsula, offers an excellent opportunity to study seismic anisotropy. Path-integrated anisotropy can be estimated most readily from shear waves that enter an anisotropic region with a known polarization, as it is the case of the SKS and SKKS. Splitting observations in orogenic regions have often, but not universally, indicated a fast axis parallel to the orogeny, which is consistent with collisional shortening of the mantle root (Silver, 1996). Our SKS measurements beneath MTE seem to confirm this result.

Publicado em:

Livro de resumos do "5.º Simpósio de Meteorologia e Geofísica da APMG", APMG2007, Peniche, Portugal (comunicação oral).

CONCEITOS FUNDAMENTAIS EM ACÚSTICA

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Instituto Superior de Engenharia de Lisboa, PT

Publicado em:

*Livro de resumos das
“1.ªs Jornadas Técnicas
de Acústica Laboral e
Ambiental & Vibrações
no Corpo Humano”,
Instituto de Soldadura
e Qualidade, Lisboa,
Portugal (comunicação
oral).*

Os Técnicos que têm a seu cargo a elaboração de Planos de Monitorização/Redução de Ruído devem possuir uma sólida formação em termos dos Conceitos Fundamentais da Acústica.

De facto, a medição e/ou previsão de níveis acústicos para posterior análise e eventual controlo, deve ser efectuada de acordo com o estabelecido na Legislação e na Normalização aplicável em vigor, sendo para tal necessário conhecer adequadamente as grandezas acústicas a monitorizar/prever, bem como a forma como estas evoluem e interagem, quer no domínio do tempo, quer no domínio do espaço, quer no domínio da frequência.

A ACÚSTICA EM PORTUGAL

Rodrigues, Carlos César

Instituto Superior de Engenharia de Lisboa, PT

A Engenharia Acústica como matéria transversal da Engenharia tem vindo a assumir no nosso País um crescimento constante e significativo na última década, nomeadamente com o aumento do número e da respectiva competência técnica das entidades e das empresas envolvidas. Para este crescimento contribuiu de forma decisiva o facto da Ordem dos Engenheiros ter criado a Especialização em Engenharia Acústica, que conta, até à presente data, com cerca de duas dezenas de Especialistas.

A Acústica hoje e os desafios para amanhã foram objecto de debate no 1º Encontro de Técnicos de Acústica do Algarve.

Publicado em:

Livro de resumos do "1º Encontro de Técnicos de Acústica do Algarve", Escola Superior de Tecnologia da Universidade do Algarve, Faro, Portugal (comunicação oral).



07

MATEMÁTICA

Anuário Científico 2007

ISEL

SHARP CONDITIONS FOR THE EXISTENCE OF SOLUTIONS OF SECOND-ORDER AUTONOMOUS DIFFERENTIAL EQUATIONS

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We prove general existence results for the autonomous equation

$$x'' = f(x)g(x'), \quad x(0) = x_0, \quad x'(0) = x_1,$$

where f and g need not be continuous or monotone. Moreover neither f nor g need be bounded around, respectively, x_0 and x_1 , thus allowing singularities in the equation. Several other basic topics such as uniqueness, continuation, extremality and periodicity are studied in our general framework.

Publicado em:

Mediterranean Journal of Mathematics, 2007, Vol. 4 N^o2, 191-214.

EXISTENCE AND LOCALIZATION OF SOLUTIONS FOR FOURTH-ORDER BOUNDARY VALUE PROBLEMS

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In this paper, we study the existence of solutions for the differential equation $u^{(4)}(t) = f(t, u(t), u''(t))$, with periodic or “simply supported” boundary conditions. We use the method of lower and upper solutions, for both the well-ordered and the reversely-ordered cases.

Publicado em:

*Electronic Journal of
Differential Equations*
2007, 127, 1-10.

VARIANCE COMPONENTS ESTIMATION IN GENERALIZED ORTHOGONAL MODELS

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The model is generalized orthogonal if the orthogonal projection matrices on the range spaces of matrices X_j , $j=1, \dots, w$, commute. Unbiased estimators are obtained for the variance components of such models with cross-nesting.

Publicado em:
*Discussiones
Mathematicae –
Probability and
Statistics, 2007, 1-2,
99-115.*

A NONCONFORMING MULTIDOMAINS METHOD FOR CONTACT PROBLEMS

Rodrigues, J.A.

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Publicado em:

*American Institute
Proceedings of
Numiform 07, Porto,
17 a 21 de Junho de
2007, pp. 1609-1614.*

With this work we present nonconforming finite elements approximation of the contact problem based on a three-fields multidomains formulation. We will show for some examples that the numerical results obtained with nonconforming multidomains techniques are qualitatively equivalent to the classic results.

The method of decomposition of domains is quite diffused as technique of resolution of differential partial equations, mainly when the system algebraic associate to the discretization of the global problem for the method of finite elements, is of high order. The use of a defined mesh globally and restricted each one of the subdomains presents some inconveniences, namely when she intend to do local refinements of the mesh. One of the techniques used on nonoverlapping decomposition of domains is the use of meshes defined independently in each subdomain, without the conformity restriction in the interfaces. The difficulty consists of assuring the global regularity of the conservatives variables. The contact problem is one of the model problems considered in the theory of variational inequality. In finite element procedures solving unilateral contact problems between two deformable bodies, each solid is often discretized independently of the other. In consequence, a finite element mesh does not coincide with the other one on the contact zone. For this reason, the constitutive or the geometrical non-linearities lead to use an incremental schema and, at each step, the up date finite element meshes. The problem is to define a convenient discrete contact condition for non-matching grids. We present domain decomposition methods within framework of mortar techniques. These domain decomposition techniques provide a more flexible approach than the standard formulations. Here, we consider a extension of the mortar finite element method formulations for a variational inequality to carry out numerical experiments associated with theoretical results already obtained.

In order to solve numerical contact problem between two elastic bodies, we have considered two finite element approximations (global and local) of order one using non-matching grids on the contact zone. It has been proved that the global approximations extends in a optimal way the classic results, obtained in the case of matching grids.

M@T- APRENDIZAGEM INTERACTIVA

Martins, S.G.

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O M@T é um livro interactivo de Cálculo disponível *online* em <http://pwp.net.ipl.pt/dec.isel/sandra.martins/mat2/mat4.htm>.

Continua em construção. Na sua realização utilizou-se *html* e *flash*.

Cada capítulo é dividido em várias secções, cada uma formada por uma explicação teórica e exemplos resolvidos, ambos apresentados de uma forma interactiva (que permite que os alunos evoluam por si, ao seu ritmo, com maior ou menor pormenor de acordo com as suas necessidades). Seguem-se mais alguns exercícios, curiosidades e finalmente um teste diagnóstico com *feedback* imediato relativo ao nível de conhecimentos do aluno, que lhe dá, ou não, a *password* que lhe permite passar para a secção seguinte.

Publicado em:

e+Calculus – Joining Educational Mathematics Workshop 1, FCUL, Lisboa, 8 a 10 de Fevereiro 2007.

GA TOPOLOGY OPTIMIZATION USING RANDOM KEYS FOR TREE ENCODING OF STRUCTURES

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Topology optimization consists in finding the spatial distribution of a certain total mass of material for the resulting structure to have some optimal property, for instance, maximization of the structure stiffness or of the fundamental eigenfrequency.

In this paper we develop a representation method based on trees to generate initial feasible individuals that remain feasible upon crossover and mutation and as such do not require any repairing operator.

Two application examples are studied: the topology optimization of structures where the objective functions is the maximization of the stiffness and the maximization of the first eigenfrequency of a plate, both cases with a prescribed material volume constraint.

Publicado em:

*WCSMO-7, 7th World
Congresses of
Structural and
Multidisciplinary
Optimization, COEX
Seoul, Korea,
21 May – 25 May
2007.*

TOPOLOGY OPTIMIZATION OF STRUCTURES USING GAS WITH RANDOM KEYS

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Topology optimization consists in finding the spatial distribution of a certain total mass of material for the resulting structure to have some optimal property, for instance, maximization of the structure stiffness and fundamental eigenfrequency, a topic currently object of intense research.

It is customary to initially discretize the continuum domain into finite elements (FE) and to define boundary conditions and applied loads on the resulting mesh. The topology optimization will consist on determining which elements will be present in the structure and which will be removed (voids).

A genetic algorithm (GA) for multi-objective topology optimization of elastic structures was developed. The genotype employed was a characteristic vector of “ones” and “zeros” indicating the presence or absence of material on a finite element mesh. As an equality constraint on volume had to be enforced, all chromosomes used generated individuals with the same volume value, *i.e.*, the same number of “ones”. This meant that to have feasible individuals the same number of “ones” and, implicitly, the same number of “zeros” has to be kept along the evolutionary process. It was thus necessary to:

I define chromosomes satisfying this propriety;

I create the corresponding crossover and mutation operators which preserves it.

In this paper we develop a method based on trees to generate initial feasible individuals that remain feasible upon crossover and mutation and as such do not require any repairing operator.

Tree encodings have received some attention in the GA literature.

As application examples we studied the topology optimization of structures where the objective functions were the maximization of the structure stiffness and the maximization of the first eigenfrequency, both cases with a prescribed material volume constraint.

Publicado em:

CMNE/CILAMCE 2007, Congresso de Métodos Numéricos em Engenharia 2007, Porto, 13 a 15 de Junho, 2007.

EXPANSÃO EM SÉRIE DE TAYLOR

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A série de Taylor é usada em inúmeros problemas; a sua demonstração é habitualmente feita em cursos elementares de Análise, usando artifícios.

Propomos uma abordagem baseada no lema de Rolle, teorema de Lagrange e, depois de estabelecer a expressão

$$f(x) = \sum_{k=0}^n \prod_{i=0}^{k-1} (\xi_i - a) f^{(k)}(a) + f^{(n+1)}(\xi_{n+1}) \prod_{i=0}^n (\xi_i - a),$$

onde posteriormente modelamos estes pontos com um modelo hierárquico, $\xi_0 = x$, e $\xi_{i|\xi_{j-1}}$ é uma variável aleatória simétrica no seu suporte (a, ξ_{j-1}) , um modelo intuitivo quando se pretende um resultado válido para qualquer função $f \in C^{n+1}$. Usando valores esperados condicionais, obtém-se de imediato o resultado tradicional.

Esta abordagem é, também, uma forma de ilustrar a extensão do teorema sobre a obtenção do valor médio da variável Y como valor médio da variável $E[Y | X]$, quando é dado um modelo hierárquico em mais do que dois passos, uma questão raramente exemplificada de forma que não seja artificiosa.

Com modelos mais gerais é possível obter expressões diversas para o resto $R(x)$, por exemplo a de Schlömilch.

Publicado em:

*Actas do XIV
Congresso da
Sociedade Portuguesa
de Estatística, Covilhã,
Portugal, Setembro de
2006, pp. 211-216.*

NON-RESPONSE AND SAMPLE SIZE

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Under the assumption that all the selected elements from a given population accept to be part of the random sample, the extension of the central limit theorem for permutable variables (Erdos and Rényi, 1959) can be used to obtain the approximate sample size that will provide the accuracy needed for the estimates of population parameters. However, in many situations, namely in sociological research, a large fraction of those selected drop out from the sample, for instance not returning questionnaires. Using Rényi's ideas on rarefaction, we investigate the effect of computing the sample size assuming an exponential or a Laplace approximation, instead of the traditional gaussian approximation.

Publicado em:

ISI 2007 Book of Abstracts of the 56th Session of the International Statistical Institute, Lisboa, 22 a 29 de Agosto de 2007, pp. 621. Artigo completo publicado no correspondente boletim electrónico (ISI Bulletin).

SYMBOLIC DYNAMICS AND CHAOTIC SYNCHRONIZATION IN COUPLED DUFFING OSCILLATOR

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In this talk we discuss the complete synchronization of two identical double-well Duffing oscillators bi-directionally coupled, from the point of view of symbolic dynamics. Working with Poincaré cross-sections and the return maps associated, the synchronization of the two oscillators, in terms of the coupling strength, is characterized.

Publicado em:

Nonlinear evolution equations and dynamical system, School and Workshop, 15-24 June 2007, Ametlla de Mar, Spain.

SYMBOLIC DYNAMICS AND SYNCHRONIZATION

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We present a brief survey of symbolic dynamics, in particular two methods to evaluate the topological entropy based on the kneading theory and on the spectral radius of the Markov transition matrix. Then we present a result for the threshold value of the coupling strength in terms of the topological entropy, to achieve synchronization of two unidirectional and bidirectional coupled unimodal and bimodal maps. Applications to the synchronization of two identical chaotic Duffing equations are given.

Publicado em:

Comunicação realizada no âmbito do PRO-GRAMA PESSOA, ações integradas de cooperação científica e técnica Luso-Francesas do projecto "Dinâmica Simbólica em iteradas de aplicações em espaços de dimensão n ($n=2,3$)", na semana de trabalho que teve lugar de 25 a 30 de Junho 2007, em Toulouse.

CHAOTIC SYNCHRONIZATION OF UNIMODAL AND BIMODAL MAPS

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We derive a threshold value for the coupling strength in terms of the growth number, to achieve synchronization of two coupled piecewise linear m -modal maps, with $m = 1$ and $m = 2$, for the unidirectional and for the bidirectional coupling. This gives us information about the synchronization of unimodal and bimodal maps. An application to the bidirectional coupling of two identical chaotic Duffing equations is given.

Publicado em:

*International
Conference on
Difference Equations
and
Applications (ICDEA),
23 a 27 Julho 2007,
em Lisboa, Portugal.*

GRAPHS, SYMBOLICS DYNAMICS AND SYNCHRONIZATION OF NETWORKS

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The synchronization of a network depends on a number of factors, including the strength of the coupling, the connection topology and the dynamical behaviour of the individual units. In this work, we relate the synchronization interval with the topological entropy in each node of a network with identical chaotic nodes. We conclude that in fully connected graphs there exists always a non empty synchronization interval. Moreover, if we fix the network topology, the amplitude of the synchronization interval decreases when the topological entropy grows. We illustrate these results taking in the nodes unimodal or symmetric bimodal maps.

Publicado em:

International Conference on Difference Equations and Applications (ICDEA), 23 a 27 Julho 2007, em Lisboa, Portugal.

SYMBOLIC DYNAMICS AND NETWORKS SYNCHRONIZATION

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In this work we use symbolic dynamics to relate the synchronization interval of a network with the topological entropy in each node. In particular, we conclude that in some graphs there exist always a non empty synchronization interval. Moreover, if we fix the network topology, the amplitude of the synchronization interval decreases when the topological entropy increases.

Publicado em:

*Proceedings of the
IEEE International
Workshop on
Nonlinear Maps and
their Applications
(NOMA'07), 13-14
December 2007, INSA,
Toulouse, France, pp.
44-47.*

SCALAR FIELD PHASE DYNAMICS IN PREHEATING

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We study the model of a massive inflaton field χ coupled to another scalar field η with interaction term $g^2\chi^2\eta^2$ for the first stage of preheating. We obtain the behavior of the phase in terms of the iteration of a simple family of circle maps. When expansion of the universe is taken into account the qualitative behavior of the phase and growth number evolution is reminiscent of the behavior found in the case without expansion.

Publicado em:

The Eleventh Marcel Grossmann Meeting On Recent Developments in Theoretical and Experimental General Relativity, Gravitation and Relativistic Field Theories (In 3 Volumes) Proceedings of the MG11 Meeting on General Relativity Berlin, Germany 23 - 29 July 2006.

TRAVEL-TIME FOR A SINGLE ORIGIN-DESTINATION

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The BRISA problem was to calculate the real time travel information using the Via-Verde (VV) technology (floating data) and automatic data for the area defined by the triangle A5 Lisboa-Cascais and A9 Estúdio-Queluz. To solve the problem we will be able to make use of the large amounts of traffic data that will soon become accessible electronically in real time; indeed there are two different information sources producing different data for the same object and context. There is a tremendous demand for simple information concerning just the travel-time for a single origin-destination and service level for a motorway section. It was suggested that we should use a Hybrid Traffic Flow Modelling to cope with this challenge.

Publicado em:

*Report of the The 60th
European Study Group
with Industry 2007.*

REPORT ON THE STEWART PLATTFORM PROBLEM

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- 2 C. de Física Teórica e Computacional, UL, Lisboa, Portugal
- 3 Dept. de Engenharia Civil, ISEL, Lisboa, Portugal
- 4 Dept. de Matemática, F. de Motricidade Humana, UT, Lisboa, Portugal
- 5 Grupo de Física Matemática, UL, Lisboa, Portugal

A Stewart platform, also known as a hexapod positioner, is a parallel manipulator using an octahedral assembly of struts. There are six independently actuated legs, where the lengths of the legs are changed to position and orient the platform. The purpose of this study was to consider the following problems:

| The forward kinematics problem: given the leg lengths, find the position and orientation, velocity and acceleration of the platform.

| The inverse kinematics problem: given the position and orientation, velocity and acceleration of the platform obtain the legs lengths dynamics.

| Provide methods to determine conditions ensuring that there are no architectural singularities for a given platform.

Publicado em:

*Livro de Resumos da
Conferência Nonlinear
Evolution and
Dynamical Systems,
L'Ametlla de Mar,
Barcelona, Espanha,
16 a 23 de Junho de
2007*

SYMBOLIC DYNAMICS AND COMPLEXITY IN A OVERLAPPING GENERATION MODEL

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- 2 Departamento de Matemática, U. Évora, Évora, Portugal
- 3 Departamento de Métodos Quantitativos, ISCTE, Lisboa, Portugal

The purpose of this paper is to study the Kaas L. and Zink S. economic model about interaction between human capital accumulation and economic growth. We use the techniques of symbolic dynamics and the kneading theory to obtain some properties (with explicit computation) of the associated discrete dynamical system. The analysis of the results allows us to understand the economics dynamics features and to distinguish different scenarios.

Publicado em:

*Livro de Resumos da
Conferência
Applications of Physics
in Financial Analysis
Dynamics, Lisboa,
4 a 7 de Julho de
2007.*

ECOLOGICAL COMPLEXITY: CHAOS IN A THREE SPECIES FOOD CHAIN MODEL

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3 Departamento de Matemática, IST, Lisboa, Portugal

The study of ecological systems has generated deep interest in exploring the complexity of chaotic food chains. The role of chaos in ecosystems is not entirely understood. One approach to have a better comprehension of ecological chaos is by analyzing it in mathematical models of basic food chains. In this article it is considered a classical chaotic food chain model from the literature. We use the theory of symbolic dynamics to study the topological entropy and the parameter space ordering of kneading sequences associated to one-dimensional maps that reproduce significant aspects of the model dynamics. The topological entropy allows us to distinguish different chaotic states in some realistic system parameter region. Another numerical invariant is introduced in order to characterize isentropic dynamics. Studying a set of maps with the same topological entropy, we exhibit numerical results about the relation between the second topological invariant and each of the control parameters in consideration. This work provides an illustration of how our understanding of ecological models can be enhanced by the theory of symbolic dynamics.

Publicado em:

*Livro de Resumos da
Conferência Nonlinear
Dynamics and Chãos:
Advances and
Perspectives,
Aberdeen, Escócia,
17 a 21 de Setembro
de 2007.*

LOW-DIMENSIONAL DYNAMICS OF A CHAOTIC FOOD CHAIN MODEL

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- 3 Departamento de Matemática, IST, Lisboa, Portugal

Publicado em:
*Livro de Resumos da
Conferência Nonlinear
Evolution and
Dynamical Systems,
L'Ametlla de Mar,
Barcelona, Espanha,
16 a 23 de Junho de
2007.*

An ecosystem is a web of complex interactions among species. With the purpose of understanding this complexity, it is necessary to study basic food chain dynamics. Although there is an elegant interpretation of ecological models in terms of chaos theory, the complex behavior of chaotic food chain systems is not completely understood. In the present work we study a specific food chain model from the literature. Using results from symbolic dynamics, we characterize the topological entropy of a Poincaré return map that replicates salient aspects of the dynamics of the model. The analysis of the variation of this numerical invariant, in some realistic system parameter region, allows us to quantify and to distinguish different chaotic regimes. This work is still another illustration of the role that the theory of dynamical systems can play in the study of chaotic dynamics in life sciences.

INTERACTION BETWEEN NESTED FACTORS

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² Dept. de Matemática, Univ. da Beira Interior, Covilhã, Portugal

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Interaction between factors that nest is introduced. The special case of three factor models in which the first crosses with the second that nests the third is discussed. An application to a grapevine experiment is presented.

Publicado em:

*Proceedings of the
56th Session of the
International Statistical
Institute, Lisboa,
22 a 29 de Agosto de
2007.*

INFERENCE FOR ESTIMABLE VECTORS IN ORTHOGONALLY SEPARATED ORTHOGONAL NORMAL MIXED MODELS

Ferreira, D.¹; Ferreira, S.¹; Ramos, P.²;
Mexia, J.³

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³ F. de Ciências e Tecnologia, Univ. Nova de Lisboa, Portugal

We present an orthogonal condition for normal mixed models that ensures that LSE for estimable vectors are BLUE and enables the construction of confidence ellipsoids for these vectors. A convenient version of the Scheffé theorem is presented and it is shown how to test, through duality, hypothesis on estimable vectors. These tests are equivalent to F tests and are unbiased.

We apply our results to a three factors mixed model.

Publicado em:

*Proceedings of the
56th Session of the
International Statistical
Institute, Lisboa,
22 a 29 de Agosto de
2007.*

ORTHOGONAL MIXED MODELS AND PERFECT FAMILIES OF SYMMETRIC MATRICES

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Mixed models associated to Commutative Jordan Algebras have Unbiased Estimators with Uniformly Minimum Variance for the relevant parameters. We now characterize the families of symmetric matrices that constitute basis for Commutative Jordan Algebras. This characterization is useful to establish association between models and algebras.

Publicado em:

*Proceedings of the
56th Session of the
International Statistical
Institute, Lisboa,
22 a 29 de Agosto de
2007.*

ANINHAMENTO GENERALIZADO PARA MODELOS DE EFEITOS ALEATÓRIOS

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2 F. de Ciências e Tecnologia, Univ. Nova de Lisboa, Portugal

Um modelo é ortogonal generalizado quando as matrizes de projecção ortogonal sobre os espaços imagem das matrizes X_i comutam. Para um modelo de efeitos aleatórios tem importância fundamental a estimação das componentes de variância. Neste trabalho pretende-se resolver tal problema para o caso de aninhamento múltiplo em que cada nível de cada factor, salvo o último, aninha um ou mais níveis do factor seguinte.

Publicado em:

*Actas do XIV
Congresso Anual da
Sociedade Portuguesa
de Estatística,
pp. 351-358.*

ERGONOMIC TOOLS IN AUTOMOBILE PRODUCT DEVELOPMENT

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- 3 Pininfarina, Itália

The goal of this tool is to reduce the development time of such a complex product as an automotive vehicle by using an iterative tool that can perform many key analyses mainly related with ergonomic considerations. Ergonomic compliance checks are manually performed in the late phase of product development with consequently changes on defined product development. We propose a tool with a 3D modeling and visualization environment to incorporate in the CAD design application, the check of ergonomics rules compliance during the design phase. This software tool will provide assistance to certify the vehicle for compliance with all governmental regulations and standards. It allows the users to access the ergonomic performance of the vehicle. All these tools will be written in the style of macro SCRIPT (Visual basic or c++), wizards and buttons will be created as well as the instructions to complete these, often very complex, tasks. Parameterization of the output geometry allows easily the update of the different vehicle parts. The developed software will be fully used in a parameterized CAD/CAS environment.

Publicado em:
*Proceedings of
International
Conference on
Ergonomics 2007,
December 3-5, 2007
em Kuala Lumpur
Malaysia.*

KNOWLEDGE MANAGEMENT IN AUTOMOBILE INDUSTRY

Ferreira, João

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Telecomunicações e de Computadores, ISEL, Lisboa, Portugal

Publicado em:
*Proceedings of IFAC
Conference on Cost
Effective Automation
in Networked Product
Development and
Manufacturing,
October 2-5, 2007 em
Monterrey NL México.*

A Knowledge Management system architecture is defined in this paper, based on the integrated CAD (computer Aided Design), knowledge repository and CSCW (Computer Supported Collaborative Work) system, for better support the design process in industry, particularly on the development of new products in automotive sector. The system provides a knowledge management system, based on specific domain ontology VCO (Vehicle Corporate Ontology) for the enterprise application integration (EAI). We define tools for knowledge management and retrieval of technical knowledge via models in new CAD environment, helping the users to perform their job.

KNOWLEDGE AND COLLABORATIVE ENVIRONMENTS DOMAIN ONTOLOGY

Ferreira, João

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Information integration in enterprises is a nightmare due to the differences in software and hardware platforms and due to syntactic and semantic differences in the schemas of the data sources. This is a well-known problem in the area of Enterprise Application Integration (EAI), where many applications have been developed for the purpose of information integration. Most current tools, however, only address the problems of (soft- and hardware) platform and syntactic heterogeneity; they fail to address semantic differences and they only support one-to-one (syntactical) mappings between individual schemas. In this paper we propose a domain ontology VCO (Vehicle Corporate Ontology) based on a UML2 specific profile for this business. This domain ontology will permit semantics mappings between different ontology and data base schemas, which conduct to EAI. From this information repository we will extract knowledge to user applications and a collaborate environment is establish.

Publicado em:

Proceedings of 2nd International Conference on Software and Data Technologies (ICSODT-2007), July 22 – 25, 2007 em Barcelona – Spain.

RETRIEVAL INFORMATION IN AUTOMOBILE DESIGN COMPANIES

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- 2 Pininfarina, Italia
- 3 C. para a Excelência e Inovação na Industria Automóvel, Porto, Portugal

In this paper we propose a novel retrieval system to deal with image, to help with valuable information the designers in their work and facilitate the system integration. This system uses a knowledge space provided by a domain ontology created based on UML2 profile and OWL. This space establishes the connection between user and application needs and a specialized database.

Publicado em:

*Proceedings of Second
International
Conference on Internet
Technologies and
Applications (ITA 07),
September 4-5 2007,
em Wrexham - North
Wales.*

Keywords: Retrieval Information, Desgin, Ontology, UML Profile.

VDML: A MODELING LANGUAGE FOR NEW VEHICLE DEVELOPMENT

Ferreira, João¹; Furini, F.²; Augusto, Sandra³

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- 2 Pininfarina, Italia
- 3 Volkswagen, Setubal, Portugal

Designing a new vehicle is a complex process as it requires close coordination and inputs from a number of disciplines in developing a number of systems and sub-systems in the vehicle that should fit within the confined vehicle space, function and provide the customers an acceptable combination of all relevant vehicles attributes. Understanding how these process interact and how they are aligned with other and process while they should supporting the operation tasks of the conception of a new vehicle at minimum time and cost. The first step to achieve this goal is to define a new UML profile (VDML language) based on the extension mechanics of UML (industry standard language) to assist business process description and consequent improvements originated from a high level vision.

Publicado em:
*Proceedings of
International
Conference on systems
Engineering and
Modeling (ICSEM'07),
20 to 23 of March
2007, Herzeliya e
Haifa, Israel.*

UML PROFILE APPLIED TO THE AUTOMOBILE INDUSTRY

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- 2 Dept. de Eng. Electrónica e Telecomunicações e de Computadores, ISEL, Lisboa, Portugal
- 3 Pininfarina, Italia
- 4 C. para a Excelência e Inovação na Indústria Automóvel, Porto, Portugal

Information integration in enterprises is a nightmare due to the differences in software and hardware platforms and due to syntactic and semantic differences in the schemas of the data sources. This is a well-known problem in the area of Enterprise Application Integration (EAI), where many applications have been developed for the purpose of information integration. Most current tools, however, only address the problems of (soft- and hardware) platform and syntactic heterogeneity; they fail to address semantic differences and they only support one-to-one (syntactical) mappings between individual schemas. We will analyze this problem in automobile industry through a specific UML derivate language and a domain ontology to find an adequate solution.

Publicado em:

*Proceedings of 9th
International
Conference on
Enterprise Information
Systems (ICEIS-2007),
June 12-16, 2007 no
Funchal-Madeira,
Portugal.*

MODELING PRODUCT ENGINEER AND MANUFACTURING ACTIVITY IN AUTOMOBILE INDUSTRY

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- 3 Pininfarina, Italia
- 4 C. para a Excelência e Inovação na Industria Automóvel, Porto, Portugal

Designing and consequent assembling of a new vehicle is a complex process as it requires close coordination and inputs from a number of disciplines in developing a number of systems and sub-systems in the vehicle that should fit within the confined vehicle space, function and provide the customers an acceptable combination of all relevant vehicle attributes. Understanding how these processes interact and how they are aligned with other while they should support the tasks involved in the conception of a new vehicle at a minimum time and cost is a difficult task. The first step to achieve this goal is the definition of a new UML profile (called VDML, Vehicle Development Modeling Language) based on the extension mechanics of UML (industry standard language) to assist business process description and profit consequent from the improvements achieved by the high level vision. To show the benefits of this new language applied to this specific business we model the engineer and manufacturing activity processes using VDML.

Publicado em:

Proceedings of EATIS 2007, Euro American Conference on Telematics and Information Systems, May 14-17, 2007 in Algarve - Portugal (ISBN # 978-1-59593-598-4).

FRAMEWORK FOR AN ADVANCED DESIGN VEHICLE PROCESS DEVELOPMENT

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- 2 Pininfarina, Italia
- 3 C. para a Excelência e Inovação na Indústria Automóvel, Porto, Portugal

Publicado em:
*Proceedings of IASTED
 International
 Conference on
 Modelling,
 Identification, and
 Control (MIC 2007),
 February 12-14, 2007
 in Innsbruck – Austria.*

The goal of this project is to reduce development time of such a complex product as a car design by using an iterative model that can perform many key analyses mainly related with homologation, occupant, mechanical packaging and ergonomic considerations. All these activities will be modeled and optimized with UML. This proposal describes a project for the development of a set of tools that automates many of the tasks associated with the feasibility process of an automobile in a CAD (Computer Aided Design) or CAS (Computer Aided Style) systems. This software tool will provide assistance to certify the vehicle for compliance with all governmental regulations and standards. It allows the users to access the ergonomic performance of the vehicle. All these tools will be written in the style of macro SCRIPT (Visual basic or c++), wizards and buttons will be created as well as the instructions to complete these, often very complex, tasks. Parameterization of the output geometry allows easily the update of the different vehicle parts. The developed software will be fully used in a parameterized CAD\CAS environment.

Keywords: UML, Modeling, Vehicle Design, CAD and Neural Networks.

ADL: AUTOMOBILE DIGITAL LIBRARY

Ferreira, João

Área Científica da Matemática –Dept. de Engenharia Electrónica e Telecomunicações e de Computadores, ISEL, Lisboa, Portugal

In this paper we explore the concept of a digital library (DL) applied to automobile industry business, taking into account the different project phases, formats, nomenclatures and ontologies available in the business. We construct an architecture that will provide uniform environment to users and application access to past experiences and rules. This will save money, reduce time and help the applications integration that is one of the most difficult problems to solve. We will concentrate in the design phase using same know-how and experience at Pininfarina and CEIIA. In this problem we have also to deal with confidentiality information issue, explore several levels of information access, ontology creation and mapping.

Publicado em:
*Proceedings of
Information
Technology,
Organizations and
Teams, 19-20 May,
Lisbon, Portugal.*

Keywords: Enterprise Application Integration, Ontology, UML, Digital Library.

SEMINÁRIO SOBRE PRÁTICAS INOVADORAS NO ENSINO DAS CIÊNCIAS E DA MATEMÁTICA NOS ESTADOS UNIDOS DA AMÉRICA

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- 2 Área Científica de Matemática, ISEL, IPL, Lisboa, Portugal

Como se ensina matemática e ciências em Harvard, MIT e outras escolas americanas?

Em Setembro de 2007, numa visita a várias universidades e centros de investigação na costa Este dos EUA, foi possível contactar com diferentes formas de ensinar ciências e matemática a alunos dos primeiros anos do Ensino Superior. Neste seminário foram apresentados os seguintes projectos:

Publicado em:

*Seminários da
Unidade de
Investigação Educação
e Desenvolvimento,
FCT UNL, Campus da
Caparica, 31 de
Outubro de 2007.*

Harvard

| Derek Bok Center – Centro para preparação e apoio pedagógico de professores e assistentes.

| Calculus Consortium – Um currículo de Cálculo inovador criado por 22 matemáticos de diversas universidades. Nesta abordagem privilegia-se a profundidade dos conhecimentos em detrimento da amplitude. A abordagem dos conceitos é feita seguindo várias vertentes: usando linguagem corrente, analiticamente, geometricamente e numericamente. Sempre que possível são utilizados exemplos da vida real. São muito valorizados os exercícios de aplicação dos conceitos.

| Peer Instruction – Um método inovador de ensino da física para turmas grandes, favorecendo uma aprendizagem activa baseado na interacção professor/aluno e aluno/aluno. Utilização de *ConceptTests* e tecnologia para obter *feedback* imediato relativamente ao grau de compreensão do conceito em estudo. Com impacto positivo na aprendizagem dos alunos.

MIT

| Teaching and Learning Lab – Preparação e apoio pedagógico de professores e assistentes.

| TEAL – Novo espaço para o ensino das ciências (utilizado por todos os alunos de Física 1 do MIT) com demonstrações, trabalho laboratorial, computadores e impacto positivo nas notas dos alunos – este projecto é baseado no que se descreve a seguir – SCALE-UP.

| TEAL Sim – Uso de simulações em Java para visualização de processos em Física.

North Carolina State University

| SCALE-UP – Uma sala de aulas diferente para o ensino das ciências desenhada para criar um ambiente de aprendizagem interativo, altamente colaborativo, *hands-on* e *computer-rich* (utilizando computadores como ferramenta de cálculo, veículo de pesquisa e de comunicação). Utiliza-se trabalho de grupo e actividades interessantes para cativar os estudantes e fazê-los obter uma melhor compreensão da matéria. Os resultados têm sido muito positivos.

RUELLE ZETA FUNCTIONS AND EXPANDING MAPS OF THE INTERVAL WITH HOLES

Rocha, J. Leonel¹; Alves, J. Ferreira²

- 1 Dept. de Engenharia Química, Área Científica de Matemática, ISEL, Lisboa, Portugal
- 2 Dept. de Matemática, Instituto Superior Técnico, Lisboa, Portugal

In this talk we discuss a class of open chaotic dynamical systems, from the point of view of dynamical zeta functions. Working with expanding maps of the interval with holes and dynamical zeta functions, we show how to compute explicitly important topological and metrical invariants of the system.

Publicado em:

*International
Conference - Progress
on Difference
Equations 2007, 31
Março a 5 Abril 2007,
em Laufen/Salzach,
Alemanha.*

MÉTODO DE DECOMPOSIÇÃO DE DOMÍNIOS PARA PROBLEMAS DE CONTACTO

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Área Científica de Matemática, ISEL, Lisboa, Portugal

Apresentaremos um método de decomposição de domínio usando a técnica de “Mortar” para a resolução de um problema de contacto. Esta técnica foi originalmente introduzida como um método não conforme para associar elementos espectrais, tendo-se revelado aplicável a várias situações tais como na associação de diferentes modelos, métodos de discretização ou triangulações não conformes ao longo das interfaces interiores do subdomínio. Aplicaremos esta técnica a uma formulação macro-híbrida de um problema de contacto sem fricção com condições bilaterais. A discretização considerada será local e independente aproveitando as características geométricas do problema, sendo a regularidade global da solução assegurada no sentido fraco através da introdução de três espaços de junção nas interfaces dos subdomínios. Baseado ainda na técnica “Mortar” apresentamos posteriormente um algoritmo do tipo Dirichlet-Neumann para a resolução de um problema de contacto sem fricção com condições unilaterais.

Publicado em:

*Livros de Resumos do
Métodos Numéricos e
Computacionais em
Engenharia - CMNE
CILAMCE 2007, Porto,
13 a 15 de Junho de
2007.*

E-ESTRATÉGIA NO ENSINO DA MATEMÁTICA

Rodrigues, J.A.

Área Científica de Matemática, ISEL, Lisboa, Portugal

Publicado em:

*Livros de Resumos do
eLearning Lisboa 07 -
EU Conference, 15 e
16 de Outubro de
2007.*

O ensino da Matemática baseado apenas numa estrutura lógica e coerente, inicia-se tradicionalmente com a apresentação formal dos conceitos, terminando nalgumas das suas aplicações, permitindo uma boa planificação da estrutura do curso, por norma baseada na apresentação predominantemente expositiva, cobrindo todos os temas da unidade curricular. No entanto, esta metodologia tem a desvantagem de ser inflexível na adaptação aos modos de ser e de pensar de cada aluno. Para a maioria dos alunos, este sistema de ensino apenas produz uma aprendizagem centrada na memorização de umas quantas fórmulas, e procedimentos, a serem esquecidos após os exames. Com esta comunicação propomos apresentar práticas de e-learning desenvolvidas no contexto do ensino da Matemática no curso de Engenharia Civil, no ISEL. Mostraremos também, a forma como estas práticas contribuem para uma melhoria da qualidade de ensino nas disciplinas de Análise Matemática I e Análise Matemática II, do curso de Engenharia Civil.

MATHEMATICS AND STATISTICS – ON THE OTHER SIDE OF THE MIRROR?

Simões, N.M.

Área de Matemática, Dept. de Engenharia Civil, ISEL, Lisboa, Portugal

1. Is Mathematics (and Statistics) a pure exquisite and abstract science, which creates a different world – on the other side of the mirror? Is it condemned to be a cultural anathema, to the amusement of a few enlightened minds? A distant island or a prickly way just made of incomprehensible formulas accessible just to a few? Another brick in the wall – as the famous Pink Floyd song? It is true that Maths is often “felt” this way: as a scaring and painful discipline, maybe because of the traditional ways of teaching and learning maths, ..., maybe because some want to impose their discretionary cathedra power by (artificially) augmenting the distance between ‘those who know’ and those who don’t (...)

2. Another look at Maths and its social responsibility:

Or is it (maths) also an instrument that has been able, along human history, to discover new solutions to old and new problems? If we pay attention to the long waves/short waves of technological evolution, we might discover the presence of maths discoveries as time goes by and in some special history’s jumps ... If we look at economic growth, where technology and knowledge have a decisive role, we discover the hidden inclusion of maths in it.

Considering that output at time t is expressed by a simple Cobb Douglas model: $Y(t) = K(t)^\alpha [A(t) H(t)]^{1-\alpha}$ here Y is the output (production), K is capital, A is the effectiveness of labour, and H is the total amount of productive services supplied by workers; and considering that both K (capital – technology) and A (the effectiveness of labour) are both implicit functions of mathematical knowledge, we get to the conclusion that, the more mathematics knowledge and the respective competencies grow, the more product grows, ... unless there is a restriction external to the model (...). At this point, we might at the one hand reflect on the implications of these theoretical deductions: Is this always true? Is all mathematical knowledge part of economic growth? Isn’t there un-useful knowledge in maths? Should we look at maths just from this strict point of view? Is growth an absolute value – is it always good? And, ... what about the trade-off growth/sustainability? The children’s story “The beauty and the beast” might

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help us comprehend this dilemma. The fact is that one might look at Maths (and knowledge) as a twofold coin:

the beauty and the beast.

The beauty is the pleasure maths gives us as a discipline to the honour of human spirit, the possibilities it develops in understanding reality, in innovating (in a broad sense), and in getting higher levels of quality of life, the beast is a metaphor to the 'disgust' maths gives to many of those who get in touch with it (Enzensberg called it "a cultural anathema") ... and also to the indirect negative effects of knowledge: knowledge might also be used as a weapon to destruction ...

The antidote to this is, we believe, in developing competencies in a broad sense – where knowledge is not partial and too specialized but holistic, and also, mainly, in developing common values as an anchor. Let's hope the beast finally transforms into a prince (as in the child story) – and aesthetics marries the effectiveness of socio-economic development!

(...)

ORIENTATIONAL DIRECTOR EFFECTS IN THE CONTINUUM THEORY OF NEMATIC LIQUID CRYSTALS

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Oriental director effects in nematic liquid crystals driven by external forces are investigated. The continuum theory of nematic liquid crystals leads to a system of non-linear differential equations to describe the spatial orientation of the director field. Analytical methods are used to solve these non-linear differential equations obtained from a modified and more convenient form of the Ericksen-Leslie partial differential equations. Some hydrodynamic limits are considered, in particular, flow regimes with small Ericksen number. Analytical solutions are presented for some boundary conditions and some physical interpretation is given.

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MÉTODOS MATEMÁTICOS EM ENGENHARIA – MODELOS EM IR

Rodrigues, José Alberto

Colecção: Caminhos do Conhecimento
Edições Colibri e Instituto Politécnico de Lisboa

Este texto dirige-se aos alunos do primeiro ano de Engenharia que pretendam adquirir ou consolidar conhecimentos em Análise Matemática, razão pela qual se adoptou um método de exposição elementar. Mais do que um manual, este livro pretende fornecer ao leitor os métodos, as ideias e as ferramentas do Cálculo Real. O desenvolvimento teórico de cada um dos assuntos foi otimizado, sendo que as demonstrações dos princípios só são exibidas quando possuem um carácter didáctico. Com este primeiro trabalho, pretende-se que o leitor adquira real entendimento do exercício resolvido e que ganhe competências na resolução de problemas práticos, formulando correctamente o problema matemático, considerando as possíveis maneiras de obter uma resposta correcta. Restringimo-nos, neste trabalho, aos problemas que admitem modelos unidimensionais. A resolução de problemas foi usada para exemplificar extensivamente os conceitos teóricos. Problemas suplementares são propostos no final de cada secção.

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