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Resumos de Artigos, Comunicações, Teses e Livros





# ENGENHARIA CIVIL

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# GESTÃO DE INTERSECÇÕES RODOVIÁRIAS – FUNCIONAMENTO EM MODELOS DE ROTUNDA

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Analisa-se a problemática da gestão das intersecções rodoviárias, numa perspectiva adaptativa destas às variações da procura, de forma a satisfazer os adequados níveis de capacidade, segurança e comodidade. Faz-se referência à necessidade de proceder ao redimensionamento das intersecções de nível, enquadrando essa evolução num contexto mais lato do que a perspectiva única do aumento de capacidade. Apresenta-se um pequeno levantamento comparativo das metodologias de referência para o dimensionamento de intersecções giratórias. Com base nestas comparações podem surgir algumas interrogações acerca das motivações por detrás da dispersão, quer das formulações teóricas, quer dos resultados práticos obtidos. Apontam-se algumas pistas prováveis para as diferenças encontradas, bem como alguns caminhos para melhorar a percepção e mitigar essas diferenças.

A gestão da infra-estrutura rodoviária assenta sistematicamente num 'confronto' entre a oferta disponibilizada e a procura (os utilizadores). Quando esse 'confronto' é pacífico e corre bem podemos afirmar que estamos numa situação de equilíbrio. No entanto, este equilíbrio é dinâmico e precário a médio/longo prazo, devido à procura de transportes ser, por um lado, uma procura derivada, dependente das cadeias de actividades dos utilizadores. Por outro lado, por ser uma procura induzida, quer através da alteração da própria oferta de infra-estrutura, quer através de outros factores, intrínsecos ou não, ao Sector dos Transportes.

No âmbito da gestão da infra-estrutura, apresentam-se algumas ideias relativas à problemática das intersecções rodoviárias não semaforizadas, quer estas se integrem em meio urbano, ou ambiente interurbano (rural). Discute-se nomeadamente a problemática da transformação das intersecções clássicas (cruzamentos de nível) em intersecções giratórias (rotundas).

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Rodoviário Português,  
Lisboa, Portugal,  
Novembro de 2004.*

# CRITERIA FOR THE USE OF FINE RECYCLED CONCRETE AGGREGATES IN CONCRETE PRODUCTION

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Conference on the Use  
of Recycled Materials  
in Buildings and  
Structures", Barcelona,  
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In many research programs, recycled aggregates from concrete have been used to produce new concrete with promising results. However, in almost all of these research programs, only the coarse aggregates have been used and it was taken for granted that the fine portion was unsuitable for this purpose.

Nevertheless, in many countries the extraction of fine natural aggregates (sand) has had tremendous environmental repercussions, namely in rivers and sea coastal areas. In Portugal, a major bridge collapse, causing the loss of nearly 70 human lives, was directly connected with the extraction of sand in inadequate quantities and location.

The present research program, in which concretes have been produced with different substitutions (10%, 20%, 30%, 50% and 100%) of natural sand with fine recycled concrete aggregates, has been divided in three parts: tune-fining the workability of the admixtures in order to keep it constant; choosing the maximum allowable substitution percentage according to performance criteria; performing a large set of laboratory tests to compare the behaviour of a concrete with that same percentage of fine recycled aggregates with the behaviour of a reference concrete produced exclusively with fine natural aggregates. In all compositions, the coarse portion is made of natural limestone aggregates.

The present paper describes the second part of this research program and the criteria used to limit the maximum replacement ratio, based on compressive strength, short-term shrinkage and water absorption by capillarity.

# DESEMPENHO MECÂNICO DE BETÕES COM INERTES FINOS RECICLADOS DE BETÃO

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A crescente dificuldade em obter agregados naturais para a execução de betão, associada aos custos ambientais e sociais que a extracção dos mesmos acarreta, levou a que se procurassem alternativas viáveis à sua substituição. Um dos caminhos tomados foi o de reaproveitar os resíduos de construção e demolição para novos agregados.

Apesar de muito trabalho já ter sido desenvolvido na substituição dos agregados grossos por seus semelhantes reciclados, a parcela fina tem sido menosprezada, em parte por alguns estudos mostrarem um desempenho pouco interessante da mesma. Apesar dos resultados previamente obtidos, julga-se notório que a obtenção de soluções alternativas às areias naturais é de extrema importância, em particular em Portugal, onde a sua extracção teve já implicações em acontecimentos tragicamente conhecidos.

Neste sentido, está em curso no Instituto Superior Técnico uma investigação que tem por objectivo averiguar a viabilidade de incorporação de inertes finos provenientes da reciclagem de betão em novos betões, com propriedades adequadas à sua utilização em estruturas de betão armado ou mesmo betão pré-esforçado. A campanha experimental está dividida em três fases distintas, nas quais são estudadas composições com diferentes percentagens de substituição (10%, 20%, 30%, 50% e 100%) e onde serão estudadas algumas características mecânicas e de durabilidade dos referidos betões.

Nesta comunicação apresentam-se os resultados obtidos no desempenho mecânico nas três fases, nomeadamente resistência à compressão, resistência à tracção e módulo de elasticidade.

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*Livro de Actas do Encontro Nacional de Betão Estrutural 2004. Porto, Portugal, Novembro de 2004.*

# INCORPORAÇÃO DE AGREGADOS FINOS RECICLADOS DE BETÃO NA PRODUÇÃO DE NOVOS BETÕES

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Congresso Nacional de  
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Dezembro de 2004.*

Na produção de betões com agregados reciclados, a parcela de finos é identificada em toda a bibliografia conhecida como aquela que conduz de uma forma mais acentuada a um aumento na água de amassadura, o que tem diversas consequências negativas no desempenho desses mesmos betões.

O principal argumento que sustenta a utilização dos agregados reciclados, a sua componente de preservação de meio ambiente, aplica-se em Portugal com particular relevância no caso das areias, como se verificou em Entre-os-Rios.

É por essa razão que está em curso no Instituto Superior Técnico uma campanha experimental conducente à elaboração de uma dissertação de Mestrado em Construção em que o objectivo é o de produzir betões com incorporação crescente de agregados finos reciclados de betão compensada, para manter o nível de trabalhabilidade, o teor em cimento e a curva granulométrica, pelo aumento da relação água/cimento efectiva, o que pressupõe a determinação prévia da absorção de água dos finos reciclados através de um ensaio e uma metodologia preconizada na literatura.

Nesta comunicação, apresentam-se os primeiros resultados desta campanha, nomeadamente a fase de acerto de relação água / cimento versus percentagem de incorporação de reciclados.

# VARIAÇÃO DOS CUSTOS DE UM EDIFÍCIO NAS DIFERENTES ZONAS SÍSMICAS.

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Com base na estrutura de um edifício construído em Lisboa, calcularam-se as armaduras dos diferentes elementos estruturais para sete níveis de acção sísmica, correspondentes a “Zona Sem Sismo”, Zonas Sísmicas D a A, Zona A’ e Zona A”, com valores dos coeficientes sísmicos iguais a 0.0, 0.3, 0.5, 0.7, 1.0, 1.25 e 1.5, respectivamente. Utilizaram-se dois programas de cálculo diferentes, um de Pórticos Planos e outro Tridimensional, para a análise estrutural e cálculo das armaduras.

Comparam-se deslocamentos, modos de vibração e frequências. Faz-se uma análise da evolução das quantidades de aço nos diferentes elementos “sismo-resistentes” da estrutura. Compara-se a evolução dos custos da Estrutura e do Edifício nas diferentes zonas sísmicas de Portugal e estimam-se os eventuais acréscimos do custo do Edifício resultantes de da adopção de coeficientes sísmicos majorados de 25% e 50% relativamente aos definidos no Regulamento de Segurança e Acções.

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*CD e Livro de Actas do 6º Encontro Nacional de Sismologia e Engenharia Sísmica, Universidade do Minho, Guimarães, Portugal, 14 a 16 de Abril de 2004.*

# INFLUÊNCIA DA ACÇÃO SÍSMICA NOS CUSTOS DE UM EDIFÍCIO

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Dimensionaram-se os diferentes elementos estruturais de um Edifício para sete níveis de acção sísmica, quantificada de acordo com o Regulamento de Segurança e Acções.

Faz-se uma análise da variação das quantidades de aço e dos custos da Estrutura e do Edifício nas diferentes zonas sísmicas.

Estimam-se os acréscimos de custo do Edifício para coeficientes sísmicos regulamentares majorados por 1,25 e 1,50.

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*CD e Livro de Actas  
do Encontro Nacional  
de Betão Estrutural  
2004 - BE2004, FEUP,  
Porto, Portugal, 17 a  
19 de Novembro de  
2004.*

# ACOMPANHAMENTO DO PROJECTO DE EXECUÇÃO DO ATERRO SANITÁRIO DE VALENÇA. VOLUME 2- COMPONENTE GEOTÉCNICA

Lopes, M.G.<sup>1,2</sup>

- 1 Laboratório Nacional de Engenharia Civil  
2 Instituto Superior de Engenharia de Lisboa

A gestão de resíduos e, nomeadamente, dos resíduos sólidos urbanos (RSU), teve um grande impulso e desenvolvimento a partir da aprovação, em Novembro de 1996, do Plano Estratégico de Gestão de Resíduos Sólidos Urbanos (PERSU) que apresenta, como grandes linhas de acção, o encerramento das lixeiras, a sua substituição por infra-estruturas adequadas de confinamento em aterro e o desenvolvimento de redes de recolha selectiva.

Neste contexto, foram identificados os responsáveis pela gestão dos RSU e definida a distribuição dos novos sistemas de gestão de RSU. Em 1997, estavam criados 29 sistemas municipais, cuja gestão, podia ser concessionada a qualquer entidade pública ou privada de natureza empresarial, e 11 sistemas multimunicipais, cuja gestão e exploração foi concessionada a empresas de capitais maioritariamente públicos, designadamente a Empresa Geral de Fomento e as autarquias. As empresas concessionárias dos sistemas multimunicipais de Vale do Minho (VALORMINHO), Vale do Lima e Baixo Cávado (RESULIMA), Baixo Cávado (BRAVAL), Gaia e St Maria da Feira (SULDOURO), Alta Estremadura (VALORLIS), Litoral Centro (ERSUC) e Algarve (ALGAR), responsáveis pelos processos de concurso para a concepção e construção dos aterros sanitários de Valença, Viana do Castelo, Braga, Vila Nova de Gaia e St Maria da Feira, Leiria, Aveiro e Figueira da Foz, Barlavento e Sotavento, pediram, em 1997, ao Laboratório Nacional de Engenharia Civil (LNEC) um estudo sobre a Avaliação da Qualidade de Aterros Sanitários de Resíduos Sólidos Urbanos, que incluía, numa primeira fase, a apreciação dos projectos e, numa segunda fase, o controlo de qualidade da construção, dos referidos aterros.

Relativamente à primeira fase da assessoria prestada pelo LNEC à empresa Valorminho – Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito da apreciação técnica do Projecto do Aterro Sanitário de Valença, foi elaborado um relatório com dois volumes. No Volume 1 foi referido o acompanhamento técnico da elaboração do projecto na sua componente ambiental, designadamente, de drenagem e tratamento de lixiviados, de produção de gases do aterro, das incidências ambientais e dos aspectos de exploração e de monitorização

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2004.*

no domínio das águas subterrâneas. Neste Volume 2 são resumidas as actividades desenvolvidas pelo LNEC no âmbito da apreciação geotécnica do projecto e indicadas as medidas suplementares ou correctivas que se afiguraram necessárias à garantia de qualidade da infra-estrutura a construir e do seu desempenho na fase de exploração. Relativamente à segunda fase da assessoria prestada pelo LNEC à empresa Valorminho – Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito do controlo de qualidade da construção do Aterro Sanitário de Valença, será igualmente elaborado um relatório final.

# CONTROLO DA QUALIDADE DA CONSTRUÇÃO DO ATERRO DE RESÍDUOS DE VALENÇA

Lopes, M.G.<sup>1,2</sup>

- 1 Laboratório Nacional de Engenharia Civil  
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A gestão de resíduos e, nomeadamente, dos resíduos sólidos urbanos (RSU), teve um grande impulso e desenvolvimento a partir da aprovação, em Novembro de 1996, do Plano Estratégico de Gestão de Resíduos Sólidos Urbanos (PERSU) que apresenta, como grandes linhas de acção, o encerramento das lixeiras, a sua substituição por infra-estruturas adequadas de confinamento em aterro e o desenvolvimento de redes de recolha selectiva.

Neste contexto, foram identificados os responsáveis pela gestão dos RSU e definida a distribuição dos novos sistemas de gestão de RSU. Em 1997 estavam criados 29 sistemas municipais, cuja gestão, podia ser concessionada a qualquer entidade pública ou privada de natureza empresarial, e 11 sistemas multimunicipais, cuja gestão e exploração foi concessionada a empresas de capitais maioritariamente públicos, designadamente a Empresa Geral de Fomento e as autarquias. As empresas concessionárias dos sistemas multimunicipais de Vale do Minho (VALORMINHO), Vale do Lima e Baixo Cávado (RESULIMA), Baixo Cávado (BRAVAL), Gaia e St Maria da Feira (SULDOURO), Alta Estremadura (VALORLIS), Litoral Centro (ERSUC) e Algarve (ALGAR), responsáveis pelos processos de concurso para a concepção e construção dos aterros sanitários de Valença, Viana do Castelo, Braga, Vila Nova de Gaia e St Maria da Feira, Leiria, Aveiro e Figueira da Foz, Barlavento e Sotavento, pediram, em 1997, ao Laboratório Nacional de Engenharia Civil (LNEC) um estudo sobre a Avaliação da Qualidade de Aterros Sanitários de Resíduos Sólidos Urbanos, que incluía, numa primeira fase, a apreciação dos projectos e, numa segunda fase, o controlo da qualidade da construção, dos referidos aterros.

Relativamente à primeira fase da assessoria prestada pelo LNEC à empresa VALORMINHO – Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito da apreciação técnica do Projecto do Aterro Sanitário de Valença, foi elaborado um relatório com dois volumes, onde foi referido o acompanhamento técnico da elaboração do projecto na sua componente ambiental (volume 1) e geotécnica (volume 2).

Neste relatório são resumidas as actividades geotécnicas desenvolvidas

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pelos LNEC relativamente à segunda fase da assessoria prestada pelo LNEC à empresa VALORMINHO – Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito do controlo da qualidade da construção do Aterro Sanitário de Valença.

# ACOMPANHAMENTO DO PROJECTO DE EXECUÇÃO DO ATERRO SANITÁRIO DE V. CASTELO. VOLUME 2- COMPONENTE GEOTÉCNICA

Lopes, M.G.<sup>1,2</sup>

- 1 Laboratório Nacional de Engenharia Civil  
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Relativamente à primeira fase da assessoria prestada pelo LNEC à empresa RESULIMA – Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito da apreciação técnica do Projecto do Aterro Sanitário de Viana do Castelo, foi elaborado um relatório com dois volumes. No Volume 1 foi referido o acompanhamento técnico da elaboração do projecto na sua componente ambiental, designadamente, de drenagem e tratamento de lixiviados, de produção de gases do aterro, das incidências ambientais e dos aspectos de exploração e de

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monitorização no domínio das águas subterrâneas. Neste Volume 2 são resumidas as actividades desenvolvidas pelo LNEC no âmbito da apreciação geotécnica do projecto e indicadas as medidas suplementares ou correctivas que se afiguraram necessárias à garantia de qualidade da infra-estrutura a construir e do seu desempenho na fase de exploração.

Relativamente à segunda fase da assessoria prestada pelo LNEC à empresa RESULIMA –Valorização e Tratamento de Resíduos Sólidos, S.A., no âmbito do controlo de qualidade da construção do Aterro Sanitário de Viana do Castelo, será igualmente elaborado um relatório final.

# CONTROLO DA QUALIDADE DA CONSTRUÇÃO DO ATERRO DE RESÍDUOS DE V. CASTELO

Lopes, M.G.<sup>1,2</sup>

- 1 Laboratório Nacional de Engenharia Civil  
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Relativamente à primeira fase da assessoria prestada pelo LNEC à empresa RESULIMA - Valorização e tratamento de Resíduos Sólidos, S.A., no âmbito da apreciação técnica do Projecto do Aterro Sanitário de Viana do Castelo, foi elaborado um relatório com dois volumes, onde foi referido o acompanhamento técnico da elaboração do projecto na sua componente ambiental (volume 1) e geotécnica (volume 2). Neste relatório são resumidas as actividades geotécnicas desenvolvidas pelo LNEC relativamente à segunda fase da assessoria prestada

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pelo LNEC à empresa RESULTIMA - Valorização e tratamento de Resíduos Sólidos, S.A. no âmbito do controlo da qualidade da construção do Aterro Sanitário de Viana do Castelo.

# MECHANICAL PERFORMANCE OF HDPE GEOMEMBRANES SEAMS AFTER SUNLIGHT EXPOSURE.

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Geosynthetic materials are increasingly used in solid waste landfills, but geosynthetic mechanical properties can change when exposed to sunlight. The experience with the evolution of mechanical performance due to UV radiation is not yet consolidated. Presently, at Laboratório Nacional de Engenharia Civil (LNEC) a research program concerning the evolution of the mechanical properties of HDPE geomembranes dual hot wedge seams exposed to sunlight during 12 years (expected service life of most Portuguese solid waste landfills) is under study. This paper presents the results of shear and peel tests in HDPE geomembranes dual hot wedge seams after 2, 3 and 5 years to sunlight exposure. The results are compared, on one hand, with those of the same specimens exposed to sunlight but covered by geotextile, and on the other hand, with those of the same specimens not exposed to sunlight. The change of tensile properties of covering geotextiles, after 3 years of sunlight exposure, is also presented. The analysis of the obtained results showed that the mechanical properties of the geomembrane seams were not affected significantly for the sunlight exposure until five years.

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# ESTUDO DA RESISTÊNCIA MECÂNICA DAS SOLDADURAS POR FUSÃO DE GEOMEMBRANAS DE POLIETILENO DE ALTA DENSIDADE EXPOSTAS AOS RAIOS SOLARES.

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Com o objectivo de estudar a evolução das propriedades mecânicas das soldaduras por fusão de geomembranas de polietileno de alta densidade expostas aos raios solares, está em curso um programa de investigação no Laboratório Nacional de Engenharia Civil, com o apoio das empresas concessionárias dos aterros multimunicipais de RSU portugueses. No presente artigo, apresenta-se e discute-se o trabalho experimental realizado, nomeadamente os primeiros resultados dos ensaios de corte e de arranque realizados sobre amostras expostas aos raios solares nos diferentes aterros de resíduos de norte a sul do país, cobertas ou não com geotêxtil, e sobre amostras não expostas. A análise dos resultados obtidos mostrou que, para o período de exposição decorrido (inferior a cinco anos), a resistência ao corte e ao arranque das soldaduras de geomembrana não foi significativamente afectada pela exposição aos raios solares.

# CORRELAÇÃO ENTRE O COMPORTAMENTO MECÂNICO DE AGREGADOS E DAS ROCHAS ORIGINAIS.

Conde, Mara do Carmo<sup>1</sup>; Gama, Dinis da<sup>2</sup>;  
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O estudo apresentado constitui a fase inicial de um trabalho de investigação destinado a estabelecer correlações entre as propriedades das rochas e dos agregados obtidos a partir destas. Para isso, começou por determinar-se os parâmetros de resistência do material rochoso tendo sido realizados ensaios de resistência à compressão uniaxial, carga pontual, ensaio brasileiro, martelo de Schmidt e durabilidade (slake durability). Em relação aos agregados, a resistência foi avaliada através de ensaios de desgaste por abrasão, utilizando o equipamento de Los Angeles. Foram seguidamente estabelecidas correlações entre os parâmetros de resistência obtidos para a rocha original e para os agregados. Estas correlações são de grande interesse por permitirem, a partir das sondagens do terreno na fase de ante-projecto de uma obra, avaliar, através de ensaios realizados na rocha, as características prováveis dos agregados que se podem obter.

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*Actas do 9º Congresso Nacional de Geotecnia, Aveiro de 19 a 23 de Abril de 2004.*

# O ENSINO DA QUALIDADE NA ENGENHARIA

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**Publicado em:**  
Congresso  
"Construção 2004" da  
FEUP.

## 1. Os desafios para a competitividade portuguesa

Constitui lugar comum dizer que a economia portuguesa tem que ser competitiva pelo lado do BOM e não pelo do BARATO.

As exigências deste padrão de competitividade obrigam a mudança de mentalidades: grande esforço na educação de base, formação profissional, interacção entre empresas e o sistema de investigação e desenvolvimento e capacidade de empreender projectos empresariais assentes na inovação, qualidade e diferente relacionamento com os mercados.

## 2. Os desafios para a Qualidade em Portugal

As mudanças que as Normas ISO 9000/2000 introduziram na Certificação em Qualidade, demonstram que não é simples evolução e sim revolução:

- os aspectos comportamentais passam a estar no cerne;
- a abordagem de Processo e a melhoria contínua, exigem atitude de incomodidade permanente;
- a liderança tem que ser mais responsável porque se mede pelo exemplo, nomeadamente na definição de objectivos;
- o que passa a contar são resultados e não "burocracia de papeis".

Contudo, não é nas Empresas Certificadas que está o problema e sim nas que o não estão.

Como conseguir que se especializem em qualidade com baixos níveis de formação em gestão dos dirigentes e quadros intermédios e muito baixos níveis de instrução dos executantes?

# “OUTPUT ONLY” ANALYSIS APPLIED ON A REINFORCED CONCRETE BUILDING, LISBON.

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The study described in this paper presents the main results of the DYNASEIS Experiment. Ambient Vibration testing was conducted on a reinforced concrete building in Lisbon, Portugal, in order to obtain the dynamic parameters of the structure, including the fundamental lateral and torsional natural frequencies of the building, as well as the corresponding damping ratios and mode shapes. Those parameters were determined using ARTeMIS extractor, a commercially available computer program, that use output-only modal identification techniques. Two independent techniques were used for modal identification and compared, peak picking (PP) method in the frequency domain and the stochastic subspace identification (SSI) method in the time domain.

A finite element model of the structure was developed in SAP2000 (version 7.1) and performed analytical modal analysis to achieve natural frequencies and mode shapes, this analytical results were compared with experimental results and presented.

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*“Proceedings” da XXII Conferência Internacional de Análise Modal (IMAC XXII), Dearborn, Michigan, EUA, Janeiro de 2004.*

# DAMAGE CHARACTERIZATION IN CONCRETE DAMS USING “OUTPUT-ONLY” MODAL ANALYSIS.

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*“Proceedings” da XXII  
Conferência  
Internacional de  
Análise Modal  
(IMAC XXII), Dearborn,  
Michigan, EUA, Janeiro  
de 2004.*

This work presents the results of dynamic measurements carried out at Cabril dam, the highest Portuguese arch dam, under operational conditions. The results observed are compared with those of a numerical model of 3D finite elements, based on the hypothesis of linear elastic behavior and by assuming that the hydrodynamic water pressure is properly simulated through associated water masses, in accordance with Westergaard’s formula. Reference must be made to the fact that the comparison of the observed response, during possible earthquakes, with the numerically calculated response will make it possible to analyse possible non-linear effects, such as for instance: the influence of the contraction joints movements and the issue related with damping for dynamic actions of different magnitudes.

In addition, the present work discusses the influence of reservoir water levels and of the thermal state on the time evolution of the fundamental parameters of the dynamic response (natural frequencies and mode shapes). The main purpose of that discussion is to define strategies that will make it possible to use results from dynamic monitoring under a continuous regimen to characterize alterations associated with phenomena of deterioration in arch dams.

# CARACTERIZAÇÃO DO COMPORTAMENTO DINÂMICO DE BARRAGENS DE BETÃO COM BASE EM ENSAIOS DE VIBRAÇÕES AMBIENTE E MODELOS NUMÉRICOS.

**Mendes, P.<sup>1</sup>; Oliveira, S.<sup>1,2</sup>; Rodrigues, J.<sup>1</sup>; Guerreiro, L.<sup>3</sup>; Baptista, M.A.<sup>1</sup>; Costa, A. Campos<sup>2</sup>**

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Neste trabalho apresentam-se resultados com os quais se pretende mostrar que actualmente já é possível caracterizar o comportamento dinâmico de grandes barragens de betão (frequências próprias e modos de vibração) com base na medição das vibrações ambiente, ou induzidas pelas actividades de exploração. Para tal é importante utilizar instrumentação adequada e uma estratégia de análise e interpretação das medições baseada na utilização conjunta de diferentes metodologias de identificação modal e de resultados de modelos numéricos que permitam simular o comportamento dinâmico do sistema barragem-fundação-albufeira. Este objectivo só pode ser conseguido com uma monitorização em contínuo, a qual permitirá também obter a resposta da estrutura a eventuais acções sísmicas.

**Publicado em:**

*Livro de Artigos do VI Encontro Nacional de Sismologia e Engenharia Sísmica, Guimarães, Portugal, Abril de 2004.*

# ANÁLISE EXPERIMENTAL PARA OBTENÇÃO DAS CARACTERÍSTICAS DINÂMICAS DO EDIFÍCIO DA PORTUGAL TELECOM NO PARQUE DAS NAÇÕES.

**Baptista, M.A.<sup>1,2</sup>; Mendes, P.<sup>1</sup>; Costa, A. Campos<sup>3</sup>;  
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Encontro Nacional de  
Sismologia e  
Engenharia Sísmica,  
Guimarães, Portugal,  
Abril de 2004.*

Este trabalho foi realizado no âmbito do projecto Dynaseis POCTI 36071-2000, cujos objectivos principais são: i) a determinação experimental de frequências próprias e modos de vibração de uma estrutura em betão armado localizada no Parque das Nações em Lisboa; ii) a elaboração do modelo numérico da estrutura e a sua comparação com os resultados experimentais; iii) a avaliação do comportamento da estrutura sob acção sísmica. Neste estudo apresentam-se os resultados dos ensaios experimentais e a comparação com o modelo numérico de elementos finitos (FEM). O edifício escolhido foi a torre da Portugal Telecom – Marconi no Parque das Nações, uma estrutura resistente em betão armado, construída sobre um solo aluvionar de elevado nível freático apresentando uma forma oval em planta e uma estrutura com lajes fungiformes. Foi elaborado um modelo numérico da estrutura em SAP2000. A identificação modal da estrutura foi realizada com base no software ARTeMIS Extractor”, versão 3.2, tendo-se utilizado as técnicas de identificação modal de decomposição no domínio da frequência (FDD – “Frequency Domain Decomposition”) e a de identificação estocástica de subespaços (SSI – Stochastic Subspace Identification). A comparação entre os resultados experimentais e os resultados do modelo numérico permitiu verificar que os ensaios de vibração ambiental permitem determinar convenientemente as características dinâmicas das estruturas para pequenas amplitudes do movimento.

# DYNAMIC BEHAVIOUR OF CONCRETE DAMS MONITORING AND MODELING.

**Mendes, P.<sup>1</sup>; Oliveira, S.<sup>1,2</sup>; Guerreiro, L.<sup>3</sup>;  
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This work presents the results of dynamic measurements carried out at Cabril dam, the highest Portuguese arch dam (132 m). The results observed are compared with those of a numerical model of 3D finite elements, based on the hypothesis of linear elastic behaviour and by assuming that the hydrodynamic water pressure is properly simulated through associated water masses, in accordance with Westergaard's formula. Reference must be made to the fact that the comparison of the observed response, during possible earthquakes, with the numerically calculated response will make it possible to analyse possible non-linear effects, such as for instance: the influence of the contraction joints movements and the issue related with damping for dynamic actions of different magnitudes.

In addition, the present work discusses the influence of reservoir water levels and of the thermal state on the time evolution of the fundamental parameters of the dynamic response (natural frequencies and modal configurations). The main purpose of that discussion is to define strategies that will make it possible to use results from dynamic monitoring under a continuous regimen, either to identify alterations associated with phenomena of deterioration in arch dams, or to study the effect of seismic actions of different magnitudes.

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XIII Conferência  
Mundial em  
Engenharia Sísmica,  
Vancouver, Canadá,  
Agosto de 2004.*

# USE OF AMBIENT VIBRATION TESTING FOR MODAL EVALUATION OF A 16 FLOOR REINFORCED CONCRETE BUILDING IN LISBON, PORTUGAL.

**Baptista, M.A.<sup>1,2</sup>; Mendes, P.<sup>1</sup>; Costa, A. Campos<sup>3</sup>; Afilhado, A.<sup>4</sup>; Oliveira, C.S.<sup>4</sup>**

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This paper presents a description of the experimental and analytical studies performed on a multi-storey office building in the newly residential and office area of Lisbon, Portugal. The building is located in sensitive alluvium soil, near Tagus river – Lisbon. This city was severely damaged by strong magnitude earthquakes e.g. 1531.26.01, 1755.11.01, 1969.02.28.

The selected building is a 16-storeyed reinforced concrete structure consisting of “oval” shaped flat plate slabs with a central rectangular rigid core. The Tower has 12 floors above ground and four basement levels. Ambient Vibration testing was conducted in order to obtain natural frequencies, mode shapes and damping ratios. Those parameters were obtained using Artemis software. A FEM model of the structure was developed using SAP2000 software. Both the experimental results as well as the analytical results are presented in this paper and compared.

This work was financially supported by FCT, Portugal, project 36071 ECM 2000.

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*Livro de Artigos da  
XIII Conferência  
Mundial em  
Engenharia Sísmica,  
Vancouver, Canadá,  
Agosto de 2004.*

# DYNAMIC MONITORING AND SAFETY ASSESSMENT OF CONCRETE DAMS.

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The recent developments of equipment for measuring vibrations and modal identification methodologies, give the possibility of developing dynamic monitoring systems for arch dams. These systems make it possible to record and analyse continuously, with the necessary accuracy, the response of arch dams to environmental noise and to seismic actions of any intensity whatsoever. Therefore, within the framework of dam safety control activities, these systems may be of high interest, namely as refers to: i) analysis of evolutionary deterioration processes; and ii) analysis of the effects of seismic actions.

This work presents the results of dynamic measurements carried out at Cabril dam, the highest Portuguese arch dam, under operational conditions. The results observed are compared with those of a numerical model of 3D finite elements, based on the hypothesis of linear elastic behaviour and by assuming that the hydrodynamic water pressure is properly simulated through associated water masses, in accordance with Westergaard's formula. Reference must be made to the fact that the comparison of the observed response, during possible earthquakes, with the numerically calculated response will make it possible to analyse possible non-linear effects, such as for instance: the influence of the contraction joints movements and the issue related with damping for dynamic actions of different magnitudes.

In addition, the present work discusses the influence of reservoir water levels and of the thermal state on the time evolution of the fundamental parameters of the dynamic response (natural frequencies and mode shapes). The main purpose of that discussion is to define strategies that will make it possible to use results from dynamic monitoring under a continuous regimen to characterize alterations associated with phenomena of deterioration in arch dams.

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*Livro de Resumos da  
IV Conferência de  
Engenharia de  
Barragens Nangiing,  
China, Outubro de  
2004.*

# AMBIENT VIBRATION TESTING AT N. Sra. DO CARMO CHURCH, PRELIMINARY RESULTS.

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The city of Lagos (Algarve, Portugal) is located in an area of moderate seismic risk. In recent years particular attention has been devoted to the historical centre of the city. The focus of this study is the evaluation of the seismic vulnerability of one of the most important historical monuments of the city: the church of N. Sra. do Carmo, built in the 16th century, destroyed by the 1755 Lisbon earthquake was partially rebuilt afterwards. To characterize the dynamic behaviour of this structure we developed a Finite Element Model (FEM) and performed a set of ambient vibration tests. In this paper we present a preliminary FEM of the structure and its comparison with experimental data. This work was developed in the framework of project CARAVELA - Instituto Politécnico de Lisboa.

**Publicado em:**

*Livro de Artigos da  
Conferência "Structural  
Analysis Historical  
Constructions", Pádua,  
Itália, Novembro de  
2004.*

# AN EDDY-DIFFUSIVITY/MASS-FLUX PARAMETRIZATION FOR DRY AND SHALLOW CUMULUS CONVECTION

Soares, P.M.M.<sup>1,2</sup>; Miranda, P.M.A.<sup>1</sup>;  
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Recently, a new consistent way of parametrizing simultaneously local and non-local turbulent transport for the convective atmospheric boundary has been proposed and tested for the clear boundary layer. This approach assumes that in the convective boundary layer the subgrid-scale fluxes result from two different mixing scales: small eddies, that are parametrized by an eddy-diffusivity approach, and thermals, which are represented by a mass-flux contribution. Since the interaction between the cloud layer and the underlying sub-cloud layer predominantly takes place through strong updrafts, this approach offers an interesting avenue of establishing a unified description of the turbulent transport in the cumulus topped boundary layer. This paper explores the possibility of such a new approach for the cumulus topped boundary layer. In the sub-cloud and cloud layer the mass-flux term represents the effect of strong updrafts. These are modelled by a simple entraining parcel, which determines the mean properties of the strong updrafts, the boundary layer height, the lifting condensation level and cloud top. The residual smaller scale turbulent transport is parameterized with an eddy-diffusivity approach that uses a turbulent kinetic energy closure. The new scheme is implemented and tested in the research model MesoNH.

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*Quarterly Journal  
of the Royal  
Meteorological  
Society, 2004, 130,  
3365-3384. (Revista ISI)*

# THE DIURNAL CYCLE OF SHALLOW CUMULUS CLOUDS OVER LAND: A SINGLE-COLUMN MODEL INTERCOMPARISON STUDY

Lenderink, G.<sup>1</sup>; Siebesma, A.P.<sup>1</sup>; Cheinet, S.<sup>2</sup>; Irons, S.<sup>3</sup>; Jones, C.G.<sup>4</sup>; Marquet, P.<sup>5</sup>; Müller, F.<sup>6</sup>; Olmeda, D.<sup>7</sup>; Calvo, J.<sup>7</sup>; Sánchez, E.<sup>7</sup>; Soares, P.M.M.<sup>8,9</sup>

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 the Royal  
 Meteorological  
 Society, 2004, 130,  
 3339-3364.  
 (Revista ISI)*

An intercomparison study for single-column models (SCMs) of the diurnal cycle of shallow cumulus convection is reported. The case, based on measurements at the Atmospheric Radiation Measurement program Southern Great Plains site on 21 June 1997, has been used in a large-eddy simulation intercomparison study before. Results of the SCMs reveal the following general deficiencies: too large values of cloud cover and cloud liquid water, unrealistic thermodynamic profiles, and high amounts of numerical noise. Results are also strongly dependent on vertical resolution.

These results are analysed in terms of the behaviour of the different parametrization schemes involved: the convection scheme, the turbulence scheme, and the cloud scheme. In general the behaviour of the SCMs can be grouped in two different classes: one class with too strong mixing by the turbulence scheme, the other class with too strong activity by the convection scheme. The coupling between (subcloud) turbulence and the convection scheme plays a crucial role. Finally, (in part) motivated by these results several models have been successfully updated with new parametrization schemes and/or their present schemes have been successfully modified.

# SENSITIVITY OF MOIST CONVECTION TO ENVIRONMENTAL HUMIDITY

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As part of the EUROCS (EUROpean Cloud Systems study) project, cloud-resolving model (CRM) simulations and parallel single-column model (SCM) tests of the sensitivity of moist atmospheric convection to midtropospheric humidity are presented. This sensitivity is broadly supported by observations and some previous model studies, but is still poorly quantified. Mixing between clouds and environment is a key mechanism, central to many of the fundamental differences between convection schemes.

Here, we define an idealized quasi-steady ‘testbed’, in which the large-scale environment is assumed to adjust the local mean profiles on a timescale of one hour. We then test sensitivity to the target profiles at heights above 2 km. Two independent CRMs agree reasonably well in their response to the different background profiles and both show strong deep precipitating convection in the more moist cases, but only shallow convection in the driest case. The CRM results also appear to be numerically robust. All the SCMs, most of which are one-dimensional versions of global climate models (GCMs), show sensitivity to humidity but differ in various ways from the CRMs. Some of the SCMs are improved in the light of these comparisons, with GCM improvements documented elsewhere.

## Publicado em:

*Quarterly Journal of the Royal Meteorological Society*, 2004, 130, 3055-3079. (Revista ISI)

# NEW MIXING LENGTH FORMULATION FOR THE PARAMETERIZATION OF DRY CONVECTION: IMPLEMENTATION AND EVALUATION IN THE COAMPS MESOSCALE MODEL.

Teixeira, J.<sup>1</sup>; Ferreira, J.P.<sup>2</sup>; Miranda, P.M.A.<sup>2</sup>; Haack, T.<sup>1</sup>; Doyle, J.D.<sup>1</sup>; Siebesma, A.P.<sup>3</sup>; Salgado, R.<sup>4</sup>; Soares, P.M.M.<sup>2,5</sup>

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 16th Symposium on  
 Boundary Layers and  
 Turbulence, 2004, 5.4,  
 1-7. (Extended  
 Abstract)*

The entrainment at the top of the planetary boundary layer (PBL) is a fundamental aspect of the dynamics of the dry convective boundary layer. A realistic parameterization of the entrainment and of the growth of the PBL in atmospheric models has been a major challenge in boundary layer research. It is well known that large-scale and mesoscale models have serious deficiencies in representing the development of the dry convective PBL (e.g. Ayotte et al. 1996; Beljaars and Betts 1993).

In Teixeira and Cheinet (2004) (hereafter TCo4) a simple mixing length formulation for the eddy-diffusivity parameterization of dry convection was proposed, in order to realistically represent the PBL evolution. The new formulation relates the mixing length ( $l$ ) to the square root of the turbulent kinetic energy ( $e$ ) and a time-scale ( $\tau$ ):  $l = \tau \sqrt{e}$ . Two different ways of determining the time-scale were analyzed in TCo4: (i) calculated as proportional to the ratio between the boundary layer height ( $h$ ) and the convective velocity scale ( $w^*$ ),  $\tau_h/w^*$ ; or (ii) taken as a constant, equal to the typical mean eddy turnover-time in a dry convective PBL,  $\tau_{PBL}$ . The simulation of dry atmospheric convection events showed that the new formulation reproduces in a realistic way the top entrainment and the overall PBL evolution. Although the approach of assuming a constant time-scale produced slightly worse results than the more physical one, it still showed a surprising robustness in its sensitivity to a spectrum of differing surface fluxes and tropospheric lapse-rates.

This new formulation has been generalized successfully for cloud-topped boundary layers, both in stratocumulus and cumulus cases (Cheinet and Teixeira 2003), in the context of one-dimensional (1D) models. In this paper we test this new mixing length formulation using the US Navy Coupled Ocean-Atmosphere Mesoscale Prediction System (COAMPSTM) that is briefly described in section 2. The new formulation is introduced in section 3. The observations and the mesoscale model results are analyzed in section 4. A discussion using 1D simulations is presented in section 5 and some conclusions in section 6.

# ARM CASE – EDMF SCHEME RESULTS

**Soares, P.M.M.<sup>1,2</sup>; Miranda, P.M.A.<sup>1</sup>; Teixeira, J.<sup>3</sup>;  
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The EDMF (Eddy-diffusivity/Mass-flux) scheme for describing the convective boundary layer is here tested against observations from the ARM dataset (Brown et al., 2002), corresponding to a diurnal cycle of a convective boundary layer with shallow cumulus development. The approach is based on the concept that in the convective boundary layer the main mechanisms of mixing are: local mixing that can be parameterised by an eddy-diffusivity scheme and non-local mixing performed by the mass-flux associated with thermals. The EDMF scheme was implemented in the research model MesoNH (Lafore et al., 1996), taking advantage of the eddy-diffusivity closure based on the TKE budget equation to parameterise the local transport by smaller eddies. In the sub-cloud and in the cloud layers the mass-flux term represents the effect of strong updrafts. These are modelled by a simple entraining rising parcel, which determines the boundary layer height and, if present, the lifting condensation level and cloud top.

**Publicado em:**

*Proceedings da 4<sup>a</sup>  
Assembleia Luso-  
Espanhola de  
Geodesia e Geofísica,  
2004, 145-146.  
(Extended Abstract)*

# TURBULENCE AND CONVECTION PARAMETRIZED BY A SINGLE APPROACH: EDMF SCHEMES

**Soares, P.M.M.<sup>1,2</sup>; Miranda, P.M.A.<sup>1</sup>; Teixeira, J.<sup>3</sup>;  
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This paper presents results from a set of different parameterisation schemes based on the eddy-diffusivity/mass-flux (EDMF) approach, which has been designed to describe the dry and shallow cumulus boundary layer. The EDMF schemes are based on scale decomposition between small scale turbulence, described by eddy-diffusivity, and thermals, described by mass-flux. Results obtained with the MesoNH model, where the different schemes are implemented, indicate improvements in the representation of the convective boundary layer, with and without cumulus. Comparisons are made against Large Eddy Simulation data, corresponding to the ARM case of a diurnal cycle of cumulus convection and a dry idealized case. The different EDMF schemes developed are designed to be implemented in models with either a first-order closures for turbulence and or with higher order closures.

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16th Symposium on  
Boundary Layers and  
Turbulence, Portland,  
Maine, USA, Agosto  
de 2004.*

# TESTING A NEW EDMF PARAMETRIZATION WITH THE ARM CUMULUS CASE

Soares, P.M.M.<sup>1,2</sup>; Miranda, P.M.A.<sup>1</sup>; Teixeira, J.<sup>3</sup>;  
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The Eddy-diffusivity/Mass-flux (EDMF) scheme for describing the convective boundary layer is tested against observations from the ARM dataset (Brown et al., 2002), corresponding to a diurnal cycle of a convective boundary layer with shallow cumulus development. The approach is based on the concept that in the convective boundary layer the main mechanisms of mixing are: local mixing that can be parameterised by an eddy-diffusivity scheme and non-local mixing performed by the mass-flux associated with thermals. The EDMF scheme was implemented in the research model MesoNH (Lafore et al., 1996), taking advantage of the eddy-diffusivity closure based on the TKE budget equation to parameterise the local transport by smaller eddies. In the sub-cloud and in the cloud layers the mass-flux term represents the effect of strong updrafts. These are modelled by a simple entraining rising parcel, which determines the boundary layer height and, if present, the lifting condensation level and cloud top.

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Abstracts of the  
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Union, Vol. 6, 04086,  
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2004.*

# HUMIDITY IMPACTS ON MOIST CONVECTION – EUROCS INTERCOMPARISON

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Under the European cloud systems project EUROCS, leading Cloud Resolving and Single Column Models have been intercompared under an idealized test-case designed to highlight sensitivities to mid-tropospheric humidity.

The Cloud-Resolving Models show mostly good agreement, with a humidity impact strong enough to witch convection between shallow and deep regimes. This CRM agreement is reinforced by numerical robustness tests. In contrast the single-column models show clear weaknesses in their response to humidity changes. The implications for mass flux and other convection schemes will be discussed.

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 European Geosciences  
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 Abril de 2004.*

# PRELIMINARY RESULTS OF A STUDY OF MAGNETIC PROPERTIES IN THE FOUM-ZGUID DYKE (MOROCCO)

Silva, P.F.<sup>1,2</sup>; Marques, F.O.<sup>3</sup>; Henry, B.<sup>4</sup>; Mateus, A.<sup>5</sup>; Lourenco, N.<sup>6</sup>; Miranda, J.M.<sup>1</sup>

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This work focuses on the study of flow and propagation of magma using rock magnetic analyses along sections across the thick Jurassic dyke of Fom-Zguid (Southern Morocco). Thermomagnetic data show that Ti-poor titanomagnetite is the main magnetic carrier. Petrographic analysis shows that the main Ti phase (ilmenite) occurs either as lamellae within spinel (center of the dyke) or as isolated grains (dyke margin). Bulk magnetic properties display distinct behavior according to distance to the dyke margin; grain size of the main magnetic carrier decreases towards the center of the dyke, while the natural remanent magnetization and the bulk magnetic susceptibility increase. Only the magnetic susceptibility ellipsoid close to the dyke margin corresponds to that usually found in thin dykes, with the magnetic foliation sub parallel to dyke margins. Maximum principal axis is in most cases either parallel or perpendicular to the intersection between the planes of magnetic foliation and dyke wall. Moreover, when this axis is perpendicular to the intersection it is associated with a more oblate magnetic susceptibility ellipsoid shape, indicating the presence of complex magnetic fabrics. The studied magnetic properties show that, in this 100m wide thick dyke, flow structures related with dyke propagation are only preserved close to the quickly cooled dyke margins.

**Publicado em:**

*Physics and Chemistry of the Earth, 29, 909-920, 2004.*

# COMPARATIVE AMS STUDY BETWEEN MESSEJANA (IBERIAN PENINSULA) AND FOUM-ZGUID (SOUTHERN MOROCCO) DYKES.

Silva, P.F.<sup>1,2</sup>; Marques, F.O.<sup>1</sup>; Miranda, J.M.<sup>1</sup>;  
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**Publicado em:**  
*Contributions to  
Geophysics and  
Geodesy, V34, pp.  
139-140, 2004.*

The Jurassic dykes of Messejana (Iberian Peninsula) and Foug Zguid (Southern Morocco) are two igneous structures that belong to an igneous province related with the opening of the Central Atlantic. In this work, magnetic, structural and petrological data are presented to characterize flow and propagation of magma in thick dykes, and correlate these dykes with the opening of the Central Atlantic. In some segments, the Foug Zguid dyke crops out with 100% of exposure, being thus possible to carry out a detailed structural work and collect full sections of oriented cores for magnetic fabric purposes. The same does not happen with the Messejana dyke because it is usually deeply weathered, which makes it difficult to carry out detailed structural and AMS work in the dyke margins.

In terms of magnetic mineralogy, the two dykes show Ti-poor titanomagnetite as the main magnetic carrier. Preliminary petrographic analysis for the two dykes shows that the main Ti phase is ilmenite, which occurs either as lamellae within spinel (center of the dyke) or as isolated grains (dyke margin). Bulk magnetic properties are similar for the two dykes. However, the possibility of sampling along cross-sections at Foug Zguid dyke allowed the identification of distinct behavior according to distance to the dyke margin. Grain size of the main magnetic carrier decreases towards the center of the dyke, while the natural remanent magnetization and the bulk magnetic susceptibility increase. These characteristics are most probably related with vertical magmatic differentiation.

In the Foug Zguid dyke, only the magnetic susceptibility ellipsoid close to the dyke margin corresponds to that usually found in thin dykes, with the magnetic foliation making a small angle with the dyke margins. Even so, in some sampled sites these first meters display a sharp difference of the interpretable magma flow, which are accompanied by distinct bulk magnetic properties. For Messejana dyke such accuracy of sampling near the margins was not possible to achieve, although it is possible to identify a well defined magnetic fabric. We recently initiate a comparative study in the Foug Zguid region of dykes with thickness varying from meter to hundred meters scale to evaluate flow.

# EVIDENCES OF TSUNAMI EPISODES AT TAGUS ESTUARY (PORTUGAL) SEDIMENTS SHOWN BY MAGNETIC MEANS.

Miranda, J.M.<sup>1</sup>; Silva, P.F.<sup>1,2</sup>; Baptista, M.A.<sup>1,2</sup>; Silvestre, P.<sup>1</sup>; Andrade, C.<sup>3</sup>; Freitas, C.<sup>3</sup>; Jordanova, D.<sup>4</sup>; Jordanova, N.<sup>4</sup>

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The Tagus estuary is located in the Portuguese western coast near the city of Lisbon and covers an area of approximately 320 km<sup>2</sup>. It is a high mesotidal that has been subject to several large tsunami invasions in the past, particularly at 1755 and 1531. In order to identify the sedimentary signature of the tsunami waves, the record of longer-term environmental changes of the Tagus salt marshes was studied, using environmentally-sensitive proxies to identify subtle changes of salinity, depth and temperature during the last 500 years. The analysis of vertical concentration profiles of non-anthropogenic elements indicates relatively homogeneous concentrations, in accordance with the dominant silty to clayey composition of the sediments. However, significant variations were detected for the K/Rb, La/Sm and Hf/Ta elemental ratios, probably representing variations of the sediment source. The major compositional breaks detected in the vertical profiles of these elemental pairs show some correlation with the nanoplankton vertical profiles of tax diversity and abundance suggesting that the relative contribution of marine water also changed through time. An attempt to refine the interpretation was made, using magnetic methods; magnetic susceptibility, natural remanent magnetization, anhysteretic remanent magnetization and high field measurements. A very detailed study (analysed by magnetic means one sample each 5 cm) of two cores taken from the estuary was made, revealing that the existence of three sediment layers, one of them characterised by two maxima of the magnetic susceptibility, clearly correlated with the geochemical and nanoplankton profiles, that were probably generated by 1755 and 1531 (AC) tsunamis waves.

## Publicado em:

*Contributions to Geophysics and Geodesy, V34, pp. 93-94, 2004.*

# COMPARATIVE AMS STUDY BETWEEN MESSEJANA (IBERIANPENINSULA) AND FOUM ZGUID (SOUTHERN MOROCCO) DYKES.

Silva, P.F.<sup>1,2</sup>; Marques, F.O.<sup>1</sup>; Miranda, J.M.<sup>1</sup>;  
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Rock and  
Environmental  
Magnetism, 9thCastle  
Meeting, Eslováquia,  
27 de Junho a 3 de  
Julho, 2004.*

The Jurassic dykes of Messejana (Iberian Peninsula) and Foug Zguid (Southern Morocco) are two igneous structures that belong to an igneous province related with the opening of the Central Atlantic. In this work, magnetic, structural and petrological data are presented to characterize flow and propagation of magma in thick dykes, and correlate these dykes with the opening of the Central Atlantic. In some segments, the Foug Zguid dyke crops out with 100% of exposure, being thus possible to carry out a detailed structural work and collect full sections of oriented cores for magnetic fabric purposes. The same does not happen with the Messejana dyke because it is usually deeply weathered, which makes it difficult to carry out detailed structural and AMS work in the dyke margins.

In terms of magnetic mineralogy, the two dykes show Ti-poor titanomagnetite as the main magnetic carrier. Preliminary petrographic analysis for the two dykes shows that the main Ti phase is ilmenite, which occurs either as lamellae within spinel (center of the dyke) or as isolated grains (dyke margin). Bulk magnetic properties are similar for the two dykes. However, the possibility of sampling along cross-sections at Foug Zguid dyke allowed the identification of distinct behavior according to distance to the dyke margin. Grain size of the main magnetic carrier decreases towards the center of the dyke, while the natural remanent magnetization and the bulk magnetic susceptibility increase. These characteristics are most probably related with vertical magmatic differentiation.

In the Foug Zguid dyke, only the magnetic susceptibility ellipsoid close to the dyke margin corresponds to that usually found in thin dykes, with the magnetic foliation making a small angle with the dyke margins. Even so, in some sampled sites these first meters display a sharp difference of the interpretable magma flow, which are accompanied by distinct bulk magnetic properties. For Messejana dyke such accuracy of sampling near the margins was not possible to achieve, although it is possible to identify a well defined magnetic fabric. We recently initiate a comparative study in the Foug Zguid region of dykes with thickness varying from meter to hundred meters scale to evaluate flow.

# EVIDENCES OF TSUNAMI EPISODES AT TAGUS ESTUARY (PORTUGAL) SEDIMENTS SHOWN BY MAGNETIC MEANS.

Miranda, J.M.<sup>1</sup>; Silva, P.F.<sup>1,2</sup>; Baptista, M.A.<sup>1,2</sup>; Silvestre, P.<sup>1</sup>; Andrade, C.<sup>3</sup>; Freitas, C.<sup>3</sup>; Jordanova, D.<sup>4</sup>; Jordanova, N.<sup>4</sup>

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The Tagus estuary is located in the Portuguese western coast near the city of Lisbon and covers an area of approximately 320 km<sup>2</sup>. It is a high mesotidal that has been subject to several large tsunami invasions in the past, particularly at 1755 and 1531. In order to identify the sedimentary signature of the tsunami waves, the record of longer-term environmental changes of the Tagus salt marshes was studied, using environmentally-sensitive proxies to identify subtle changes of salinity, depth and temperature during the last 500 years. The analysis of vertical concentration profiles of non-anthropogenic elements indicates relatively homogeneous concentrations, in accordance with the dominant silty to clayey composition of the sediments. However, significant variations were detected for the K/Rb, La/Sm and Hf/Ta elemental ratios, probably representing variations of the sediment source. The major compositional breaks detected in the vertical profiles of these elemental pairs show some correlation with the nanoplankton vertical profiles of tax diversity and abundance suggesting that the relative contribution of marine water also changed through time. An attempt to refine the interpretation was made, using magnetic methods; magnetic susceptibility, natural remanent magnetization, anhysteretic remanent magnetization and high field measurements. A very detailed study (analysed by magnetic means one sample each 5 cm) of two cores taken from the estuary was made, revealing that the existence of three sediment layers, one of them characterised by two maxima of the magnetic susceptibility, clearly correlated with the geochemical and nanoplankton profiles, that were probably generated by 1755 and 1531 (AC) tsunamis waves.

## Publicado em:

*New trends in geomagnetism, paleo, rock and environmental magnetism, 9th Castle Meeting, Eslováquia, 27 de Junho a 3 de Julho, 2004.*

# MAGNETIC AND SEDIMENTARY RECORDS OF MIRA RIVER (PORTUGAL).

Silva, P.F.<sup>1,2</sup>; Freitas, M.C.<sup>3</sup>; Andrade, C.<sup>3</sup>; Gama, C.<sup>4</sup>; Silvestre, P.<sup>2</sup>; Miranda, J.M.<sup>1</sup>

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April, 2004.

The Mira estuary is located in the SW Portuguese coast, 110km south of Lisbon. The river and main tributaries are deeply incised in Late Paleozoic Flysch and show a flat-floored cross section, where sediment deposited as sea-level rose since the Late Glacial. In the Corgo do Porto alluvial plain a borehole was driven to circa 28m below surface, reaching basement and yielding a continuous core which sampled the Holocene and the Late Pleistocene infill. This core has been studied for magnetic properties and sedimentology. Three main sedimentary units have been recognized, resting over bedrock, which extends below 27.5m. The basal unit A (0.69 – 27.5m) is made of barren and coarse grained detrital sediment. Its lower section (23.5-27.5m) consists of weathered shale and gravel; in the upper section (23.5 – 20.69m) the sediment ranges from gravelly sand to gravelly or sandy mud. The basal unit is interpreted as representing terrestrial sedimentation, free of marine influence and contemporaneous of the Late Pleistocene-Early Holocene; its lower section may correspond to scree and colluvium while the upper section corresponds to colluvial and alluvial, high-energy deposits. The intermediate unit B (20.69 – 2.88m) consists of a monotonous muddy sequence containing marine to brackish shell debris and whole mollusc shells. This sediment accumulated between circa 9000 and 4000 BP under variable marine influence in a transgressive context. In the upper unit C (2.88m – surface) the lower 1m is essentially sandy (coarse sand or muddy sand) with interbedded sandy mud and contains shell debris and lithoclasts; the topmost sediment is exclusively muddy, with few shell fragments at its base and abundant plant debris and charcoal further upcore. This unit represents downriver progression of a siltation front; the topmost sediment is interpreted as a freshwater floodplain deposit, occasionally affected by extreme tides, while the underlying section shows some restricted marine influence rapidly decreasing upcore. High magnetic field measurements reveal the presence of ferromagnetic minerals in variable concentrations. The measurement of the mass magnetic susceptibility ( $\chi$ ) clearly shows six sedimentary intervals with contrasting values: both the basal and top intervals match sediment units A and

C, while unit B may be subdivided. The ratio between Anhysteretic remanent magnetization and  $\chi$  and hysteresis parameters are consistent and identify nine sedimentary intervals. Magnetic results improve the capacity to discriminate sedimentary signatures and indicate changes in sediment source; magnetic properties proved to be sensitive to marine/fluvial influence.

# MAGNETIC PROPERTIES OF A DOURO MUDDY PATCH CORE (NORTHERN PORTUGUESE CONTINENTAL SHELF).

Silvestre, P.<sup>1</sup>; Silva, P.F.<sup>1,2</sup>; Drago, T.<sup>3</sup>; Silveira, T.<sup>4,5</sup>; Jordanova, N.<sup>6</sup>; Jordanova, D.<sup>6</sup>; Miranda, J.M.<sup>1</sup>

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Nice, France, 25 –30  
April, 2004.

To evaluate recent sedimentation characteristics changes, magnetic and sedimentological analyses were performed on a gravity core 3.70m long located at the muddy complex offshore Douro river, on the northern portuguese continental shelf. The core was collected during an IGM (Geological and Mining Institute of Portugal) mission on board the Poseidon vessel, in the year of 2002. Sedimentological analysis indicates the existence of three sedimentary units for the last 1400 years. The lowest one, unit A (3.70-3.30m), is very well individualised: it is the coarsest unit, it has the highest values of carbonates and presents the lowest organic matter contents. The other two units are quite similar. However, a limit at 1.50m depth can be considered: between 3.30m and till this level, Unit B is characterised by high mud and organic matter content. Above 1.50m and till the top, Unit C present lower mud and organic matter content. Magnetic measurements (magnetic susceptibility, Natural Remanent Magnetization – NRM, Anhysteretic Remanent Magnetization – ARM and high field) shows the presence of the same three units. In terms of mineral magnetic classes, Unit A, presents a considerable contribution of the paramagnetic minerals for the magnetic susceptibility signal, around 50%, while for the rest of the core 90% of the signal is dominated by ferromagnetic minerals. Thermomagnetic (Curie temperature around 580°C), Isothermal Remanent Magnetization (saturation reached for applied fields around 200mT) and hysteresis experiments are in agreement with magnetite being the main magnetic carrier. ARM measurements display similar pattern along the core, which indicates similar physics characteristics of the main ferromagnetic carrier. The study of magnetic susceptibility reveal an evolution of the concentration of magnetite from the base to the top of the core, where it is possible to observe a significant but regular increase of the susceptibility from 3.60 to 2.70m. From this level to the top the values display the same slightly decrease, although, between 2.70 and 1.50m (unit B), can be observable an oscillation of the values around the mean trend. This limit at 1.50m is also evidenced when we plot remanent ratio along the core, showing higher and stable values to the unit of the top. The inclination of NRM is very stable, around 55 degrees, from units A and B, while for Unit C, an irregular pattern is observed.

# MAGNETIC CHARACTERIZATION OF TAGUS ESTUARY(PORTUGAL) SEDIMENTS.EVIDENCE FOR TSUNAMI EPISODES?

Silva, P.F.<sup>1,2</sup>; Andrade, C.<sup>3</sup>; Baptista, M.A.<sup>1</sup>; Freitas, C.<sup>3</sup>; Silvestre, P.<sup>2</sup>; Miranda, J.M.<sup>2</sup>

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The Tagus estuary is located in the Portuguese western coast near the city of Lisbon and covers an area of approximately 320 km<sup>2</sup>. It is a high mesotidal that has been subject to several large tsunami invasions in the past, particularly at 1755 and 1531. In order to identify the sedimentary signature of the tsunami waves, the record of longer-term environmental changes of the Tagus salt marshes was studied, using environmentally-sensitive proxies to identify subtle changes of salinity, depth and temperature during the last 500 years. The analysis of vertical concentration profiles of non-anthropogenic elements indicates relatively homogeneous concentrations, in accordance with the dominant silty to clayey composition of the sediments. However, significant variations were detected for the K/Rb, La/Sm and Hf/Ta elemental ratios, probably representing variations of the sediment source. The major compositional breaks detected in the vertical profiles of these elemental pairs show some correlation with the nanoplankton vertical profiles of tax diversity and abundance suggesting that the relative contribution of marine water also changed through time. An attempt to refine the interpretation was made, using magnetic methods. A very detailed study of two cores taken from the estuary was made, revealing that the existence of three sediment layers, one of them characterised by two maxima of the magnetic susceptibility, clearly correlated with the geochemical and nanoplankton profiles, that were probably generated by 1755 and 1531 (AC) tsunamis waves.

#### Publicado em:

4<sup>a</sup> Assembleia Luso-Espanhola de Geodesia e Geofísica, Figueira da Foz, Portugal, 3-7, Fevereiro de 2004.

# ANÁLISE MAGNÉTICA DE UM CORE DA PLATAFORMA DO DOURO.

**Silvestre, P.<sup>1</sup>; Silva, P.F.<sup>1,2</sup>; Drago, T.<sup>3</sup>; Miranda, J.M.<sup>1</sup>**

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**Publicado em:**  
*4<sup>a</sup>Assembleia Luso-  
 Espanhola de  
 Geodesia e Geofísica,  
 Figueira da  
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 Fevereiro de 2004.*

During a campaign in the vessel Poseidon, a gravity corer with 3.67m was recovered at the Douro Platform (Portugal). The work here presented is focused magnetic characterization of such corer. Magnetic susceptibility ( $\chi$ ), Natural Remanent Magnetization, Anhysteretic Remanent Magnetization and high field measurements, were used for a preliminary characterization of the corer. Such results reveal the presence of three distinct levels of sedimentation for the last 1400 BP years. Although the magnetic carrier at base of the core belongs to a paramagnetic class, until approximately 2.70m, the rest upper part of the core presents ferromagnetic minerals as the main magnetic carrier. Such segment of the core, display a gradual decrease of  $\chi$  although oscillations around an average value are observed for the interval between 2.70 and 1.50.

# RESULTS OF A PRELIMINARY STUDY OF MAGNETIC PROPERTIES IN THE FOU-MZGUID (MOROCCO) AND MESSEJANA DYKES (PORTUGUESE SEGMENT).

Silva, P.F.<sup>1,2</sup>; Marques, F.O.<sup>1</sup>; Henry, B.<sup>3</sup>; Mateus, A.<sup>4</sup>; Lourenço, N.<sup>5</sup>; Miranda, J.M.<sup>1</sup>; Vegas, R.<sup>6</sup>

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This work focuses on the study of flow and propagation of magma using rock magnetic analyses along sections across the thick Jurassic dykes of Foum-Zguid (Southern Morocco) and Messejana (Portuguese segment). Thermomagnetic data show that Ti-poor titanomagnetite is the main magnetic carrier for both dykes. Petrographic analysis shows that the main Ti phase (ilmenite) occurs either as lamellae within spinel (core of the dyke) or as isolated grains (dyke rim). For Foum-Zguid dyke bulk magnetic properties display distinct behavior according to distance to the dyke rim; grain size of the main magnetic carrier decreases towards the core of the dyke, while the natural remanent magnetization and the bulk magnetic susceptibility increase. Only the magnetic susceptibility ellipsoid close to the dyke rim corresponds to that usually found in thin dykes, with the magnetic foliation parallel to dyke borders. Maximum principal axis is in most cases either parallel or perpendicular to the intersection between the planes of magnetic foliation and dyke wall. Moreover, when this axis is perpendicular to the intersection it is associated with a more oblate magnetic susceptibility ellipsoid shape, indicating the presence of complex magnetic fabrics. The studied magnetic properties show that, in the studied thick dyke, flow structures related with dyke propagation are only preserved close to the fast cooled dyke rims. The known outcrops of Messejana dyke reveal serious problems when we intent to infer the petrofabric related with magma flow by magnetic means.

## Publicado em:

*4<sup>a</sup> Assembleia Luso-Espanhola de Geodesia e Geofísica, Figueira da Foz, Portugal, 3-7, Fevereiro de 2004.*

# USE OF AMBIENT VIBRATION TESTING FOR MODAL EVALUATION OF A 16 FLOOR REINFORCED CONCRETE BUILDING IN LISBON, PORTUGAL.

Baptista, M.A.<sup>1,2</sup>; Mendes, P.<sup>1</sup>; Campos Costa, A.<sup>1,3</sup>;  
Sousa Oliveira, C.<sup>4</sup>; Afilhado, A.<sup>1,2</sup>, Silva, P.<sup>1,2</sup>

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This paper presents a description of the experimental and analytical studies performed on a multi-storey office building in the newly residential and office area of Lisbon, Portugal. The building is located in sensitive alluvium soil, near Tagus river – Lisbon. This city was severely damaged by strong magnitude earthquakes e.g. 1531.01.26, 1755.11.01 and 1969.02.28.

The selected building is a 16-storeyed reinforced concrete structure consisting of “oval” shaped flat plate slabs with a central rectangular rigid core. The structure has 12 floors above ground and four basement levels. Ambient Vibration testing was conducted in order to determine natural frequencies, mode shapes and damping ratios. Those parameters were obtained using Artemis software. A FEM model of the structure are presented in this paper and compared.

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on Earthquake  
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Canada, August, 1-6,  
2004.

# A CASE OF SOIL SLIDING IN THE PATHOLOGY OF A RETAINING STRUCTURE

**Matos e Silva, J.**

Gapres, S.A. / I.S.E.L., Lisbon, Portugal

## ABSTRACT

Sesimbra is a village located on the Portuguese West coastline 70 km South of Lisbon.

It is a site of high cliffs, overlooking the sea, mainly formed by clays. The rainwater that penetrates the soil through permeable layers originates the clays sliding.

Recent construction site in the area started with the execution of a retaining wall with counterforts.

Some time later after a long rainy period the soil sliding created a high earth pressure on the retaining wall that originated the separation between the wall and its counterforts.

The paper describes the pathology and its repair.

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Conference on  
Case Histories in  
Geotechnical  
Engineering  
April 13-17, 2004-04-10  
New York,  
NY Session 5*

# UM EXEMPLO SIGNIFICATIVO DE UTILIZAÇÃO DE PAREDES MOLDADAS ANCORADAS - O EURO STADIUM

## A SIGNIFICANT EXAMPLE OF DIAPHRAGM WALLS – THE EURO STADIUM

**Matos e Silva, J.**

Gapres/I.S.E.L., Lisboa, Portugal

### RESUMO

Refere-se o caso duma parede moldada ancorada, com cerca de 800,0 m de perímetro e altura variando entre os 11,5 m e os 21,5 m, correspondente à contenção periférica do empreendimento Euro Stadium, localizado junto ao Estádio Municipal de Coimbra.

Aborda-se o seu dimensionamento e os principais aspectos construtivos.

### ABSTRACT

The Euro Stadium diaphragm walls, with a total length of about 800,0m and with an height varying between 11,5m and 21,5m, located near the Coimbra Stadium, are referred. Design and construction aspects are analysed.

**Publicado em:**

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de Geotecnia, Aveiro,  
2004*

# REVESTIMENTOS DE IMPERMEABILIZAÇÃO DE COBERTURAS EM TERRAÇO COM BASE EM MEMBRANAS PREFABRICADAS. COMPORTAMENTO DE JUNTAS DE SOBREPOSIÇÃO

Gonçalves, Manuela

**Mestrado em:** Construção

**Grau Concedido por:** IST – Universidade Técnica de Lisboa

**Orientadores:** Jorge Manuel Grandão Lopes

**Provas Concluídas em:** 1 de Junho de 2004

A cobertura é o elemento da envolvente exterior do edifício responsável pela vedação superior do espaço habitável. A sua função é complexa e importante porque, relativamente à dos restantes elementos da envolvente os agentes atmosféricos nela actuam mais directa e intensamente.

É o caso da chuva que cai sobre as coberturas geralmente com impacto directo e é susceptível, em especial nas coberturas em terraço, de conduzir a manifestações de humidade nos edifícios. Consequentemente, pode levar à ocorrência de anomalias capazes de impedir a total satisfação das mais elementares exigências de habitabilidade das edificações.

Apesar disso, as coberturas em terraço têm características funcionais e formais que em muitos casos as recomendam ou impõem. No entanto, a constatação frequente do comportamento deficiente deste tipo de cobertura, quase sempre resultante de erros ou descuidos do projecto ou da execução, tem desprestigiado indevidamente o seu uso. Daí reconhecer-se a necessidade de discutir, esclarecer e divulgar as soluções de concepção, constituição e pormenorização construtiva dos sistemas de impermeabilização capazes de conferirem um bom desempenho às coberturas em terraço.

Entre os vários tipos de sistemas de impermeabilização de coberturas em terraço usados em Portugal, começam a ter uma utilização crescente os sistemas fixados mecanicamente de camada única, ou seja, aqueles que na zona corrente da cobertura são formados por uma única membrana, fixa pontual ou linearmente ao suporte por peças apropriadas. Contudo, o desempenho destes sistemas é fortemente condicionado pelo comportamento das ligações entre membranas, isto é, pelo comportamento das suas juntas de sobreposição. Assim, esta dissertação pretendeu contribuir para um melhor conhecimento deste tipo de sistemas de impermeabilização através da avaliação do comportamento das respectivas juntas de sobreposição.

# OBRAS SUBTERRÂNEAS: IMPERMEABILIZAÇÃO E DRENAGEM ASSOCIADA

**Justo, João Lourenço**

**Mestrado em:** Construção

**Grau Concedido por:** IST – Universidade Técnica de Lisboa

**Orientadores:** Maria da Graça Alfaro Lopes e Jorge Manuel Lopes de Brito

**Provas Concluídas em:** 27 de Outubro de 2004

O facto de não existir em Portugal documentação específica sobre a impermeabilização e drenagem associada de obras subterrâneas, gerou a necessária motivação para a selecção deste tema, acrescida ainda pelas inúmeras dificuldades vividas e sentidas pelo autor nos últimos oito anos, enquanto responsável pela realização de diversas obras do género.

Contrariamente ao que seria espectável, as dificuldades mais comuns que surgem na concretização dos trabalhos de impermeabilização têm-se mantido nos últimos anos. Por isso, o presente trabalho tem por objectivo indicar os principais aspectos a ter em consideração no projecto e na execução das diversas actividades inerentes ou interligadas ao sistema de impermeabilização e drenagem associada de obras subterrâneas, de modo a minimizar ou evitar problemas futuros, decorrentes de erros de projecto, de execução e de controlo de qualidade dos materiais e da sua instalação.

É realçada a importância da instalação adequada dos geotêxteis, geomembranas e geocompósitos contemplados nos sistemas de impermeabilização e drenagem associada das obras subterrâneas, de modo a assegurar a durabilidade estimada para as mesmas, sem desvios das condições de operacionalidade para que foram projectadas. São também descritas as tecnologias de instalação adaptadas para os sistemas apresentados e o equipamento disponível para a sua concretização, muito embora as plataformas automáticas não estejam disponíveis entre nós em face do número de obras subterrâneas, da sua tipologia e métodos de trabalho não justificarem o investimento. A metodologia adoptada na elaboração do trabalho assentou em seis fases distintas: recolha de informação técnica sobre a matéria, estudo dos métodos construtivos das estruturas e sua relação com a geologia do terreno; selecção e especificação dos materiais mais adaptados; soluções de impermeabilização e drenagem associada; processos construtivos e suas exigências (metodologia de instalação); controlo de qualidade.





02

# ENGENHARIA DE ELECTRÓNICA DE TELECOMUNICAÇÕES E DE COMPUTADORES

Anuário Científico 2004  
ISEL



# A COMPREHENSIVE ANALYSIS OF IMD BEHAVIOR IN RF CMOS POWER AMPLIFIERS

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- 4 Instituto de Telecomunicações, IST, Lisboa, Portugal

A comprehensive analysis of nonlinear intermodulation distortion (IMD) behavior in RF CMOS power amplifiers (PA) was developed. Separate analyses were developed presented for weak- and large-signal operation regimes. Especially, a new analytical large-signal IMD analysis method was developed that allows the mechanisms dominant for IMD generation to be identified and their individual contributions to be studied. By combining these analyses, typical IMD versus input power characteristics of MOSFET Pas can be predicted and understood for different classes of operation. Various measurements made on a 950 MHz RF CMOS PA were used to demonstrate typical behavior and validate the proposed theory. Prediction of IMD using a standard CMOS transistor model was also evaluated and shown a good agreement with the measurements.

**Publicado em:**

*IEEE Journal of Solid-State Circuits*, vol. 39, no. 1, pp. 24 - 34, Jan. 2004

# MOTION TRACKING IN MANIFOLDS WITH TANGENT BUNDLE APPROXIMATION

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IFAC Symposium on  
Non-Linear Control  
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2004), Stuttgart, 2004,*

In multi-dimensional tracking problems, the parameters to track are often restricted to a manifold embedded in observation space. Learning the manifold shape is useful for dimensionality reduction, lightening the computational load and simplifying the related problem of learning the dynamics. For manifolds with arbitrary topology, learning the shape from noisy scattered data presents several difficulties. This paper presents a geometric approach that addresses such difficulties. The proposed Tangent Bundle Approximation (TBA) algorithm is valid for arbitrary manifold dimension and topology. An approximation of the tangent bundle is computed, making it possible to estimate a set of manifold charts. This geometric information is then used to estimate the trajectory dynamics with a standard spline algorithm. Experimental results are presented for facetracking based on a real video sequence. The proposed method is general in scope and can be applied in any tracking problem, provided that the manifold restriction is verified.

# P-I-N FLEXIBLE IMAGING DEVICES WITH OPTICAL READOUT

Louro, P.<sup>1</sup>; Vieira, M.<sup>1</sup>; Fernandes, M.<sup>1</sup>; Schubert, M.<sup>2</sup>.

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Large area two terminal p-i-n image sensors deposited on plastic substrates were produced at low temperatures (110 degrees C) by PECVD and compared with similar sensors deposited on glass substrates. The same sensing element structure ZnO:Al/p(SiC:H)/i(Si:H)/n(SiC:H)/Al was used in all devices although with different resistivities of the front contact. In this work the efforts are focused mainly on the optimization of the output characteristics of the sensor when fabricated on plastic substrates. The role of the sensor configuration, front contact resistivity and readout parameters on the image acquisition process is analyzed. The optical-to-electrical transfer characteristics show reasonable quantum efficiency under a red light pattern, broad spectral response, and reciprocity between light and image signal. First results show that the sensors deposited on flexible substrate present smaller light to dark sensitivity than those deposited on glass. In both, the non ohmic behavior of the transparent conductive oxide front contact blocks the carrier collection and leads to a surprising linear dependence of the image signal on the applied voltage. (c) 2004 Elsevier B.V. All rights reserved.

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 ENCE BV, PO BOX 211,  
 1000 AE AMSTERDAM,  
 NETHERLANDS IDS  
 Number: 906DS ISSN:  
 0925-3467

# STACKED A-SIC : H OPTICAL TRANSDUCERS: THE INFLUENCE OF THE SENSING MATERIAL

**Louro, P.; Fernandes, M.; Rodrigues, I.;  
Fantoni, A.; Macarico, A.; Vieira, M.**

ISEL, Elect Telecommun & Comp Dept, Lisbon, Portugal

The aim of this work is to optimise the sensing a-Si alloy material characteristics in order to improve the performance of large area single and stacked p-i-n sensors for macroelectronic applications.

The efforts are focused mainly on doped n- and p-type layers at high and low doping levels with and without carbon, as well as in the intrinsic layer thickness and composition. The structural and optoelectronic properties of the single layers were determined through infrared and visible spectroscopy, temperature-dependent conductivity, and were complemented by CPM measurements. Junction properties, carrier transport, photogeneration and collection efficiency are investigated from dark and illuminated current-voltage characteristics and spectral response measurements, with and without additional background illumination and under different light bias conditions.

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FORUM II 455-456:  
81-85, 2004  
Book Series: MATERIALS  
SCIENCE FORUM  
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Fortunato E, Ferreira I,  
Dias C Publisher:  
TRANS TECH  
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# DYNAMIC CHARACTERIZATION OF LARGE AREA IMAGE SENSING STRUCTURES BASED ON A-SIC : H

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**2** Univ Nova Lisboa, Fac Ciencias & Tecnol, P-2825 Monte De Caparica, Portugal

In order to evaluate the sensor capabilities is necessary to perform a response time characterization. This work focuses on the transient response of such sensor and on the influence of the carbon contents in the doped layers. A set of devices with different percentage of carbon incorporation in the doped layers is analyzed by measuring the scanner-induced photocurrent under different bias conditions, (ranging from  $-5V$  to  $1V$ ) in order to evaluate the response time. The forward bias region is of major interest since controlled color separation can be achieved for voltages close to  $V_{oc}$ . Results show that the scanner induced photocurrent has a maximum for chopping frequencies around  $1kHz$ , while the image response time is expected to be less than  $100 \mu s$ , depending on the bias voltage. As conclusion the dynamic properties of the sensor show that the image acquisition can be performed at frame rates close to the usually used for commercial image acquisition applications, as proven by a 100 lines image at 10 fps obtained in the laboratory.

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 Number: BAF50 ,ISSN: 0255-5476  
 ISBN: 0-87849-941-5

# HIGH SENSITIVE IMAGE SENSORS BASED ON A TANDEM LASER SCANNED PHOTODIODE

**Vieira, M.; Fernandes, M.; Louro, P.; Fantoni A.;  
Rodrigues, I.**

ISEL, Elect Telecommun & Comp Dept, ISEL, Lisbon, Portugal

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ADVANCED MATERIALS  
FORUM II 455-456: 91-  
95, 2004 Editor(s):  
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MATERIALS SCIENCE  
FORUM, IDNumber:  
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941-5

In this work the efforts are focused mainly on the design of the structure and its role on sensor performance. We use different doped and intrinsic layers with different thickness and composition. The structural and optoelectronic characterisation of the single layers is presented. Junction properties, carrier transport and photogeneration are investigated from dark and illuminated current-voltage characteristics and bias dependent spectral response. The role of the design of the sensing element, the doped layer composition and thickness, the read-out parameters (applied voltage and scanner wavelength) on the image acquisition and the colour detection process are analysed.

A physical model is presented and supported by a numerical simulation of the output characteristics of the sensor. Preliminary results show the possibility of tailoring an a-SiC:H stacked heterostructure in order to optimise the tandem device as an image and colour recognition sensor.

# A GENERIC AGENT MODEL ALLOWING A CONTINUOUS CHARACTERIZATION OF EMOTION

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Departamento de Engenharia de Electrónica e Telecomunicações e  
de Computadores, ISEL, Lisboa, Portugal

Research on emotional phenomena progressively reveals a view of emotion as a dynamic process intrinsic to cognition. However, to adopt this view for agent modelling we need to go beyond the classical emphasis on the structural aspects of emotion and its assessment through verbal labels. In this paper we try to contribute to that aim by presenting a view that unifies emotion and cognition as two symbiotically integrated aspects of intelligent behaviour. The proposed models form a conceptual framework for cognitive modelling that is independent of the architectural organization of the agents, making possible to describe emotional phenomena in a concise way and to model agents of different types and levels of complexity, and where emotion is characterized as having a continuous nature.

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*Proceedings of the  
17th European  
Meeting on  
Cybernetics and  
Systems Research,  
Abril 2004*

# INTERNAL ION MOLECULE REACTIONS INSIDE CLUSTERS INDUCED BY LASER RADIATION.

**Frazão, J.M.A.<sup>1</sup>; Lourenço, J.M.C.<sup>2</sup>; Cunha, M. Áurea,<sup>3</sup>; Bhatt, M.L.<sup>2</sup>; Moutinho, A.M.C.<sup>2</sup>**

**1** Dept. de Eng. de Electrónica e Telecomunicações e de Computadores I.S.E.L

**2** CeFITec, Dept. de Física, Faculdade de Ciências e Tecnologia (U.N.L.)

**3** Departamento de Física, Instituto Superior Técnico (U.T.L.)

It is well known that molecular clusters are suitable systems to study elementary molecular reacting processes between a small and a controlled number of molecular species in presence.

In previous studies, we have reported different mechanisms involved in internal clusters ion molecular reactions (ICIMR), triggered when molecular clusters are ionized by electron impact [1,2]. We intend to continue and compare the study of these reactions replacing the electron impact ionization of the neutral clusters by a multiphoton ionization process.

The preliminary time of flight mass spectra of ionic species induced by multiphoton ionization of OCS neutral clusters will be presented. This work is part of the project POCTI/33244/FIS/2000 of the Fundação para a Ciência e a Tecnologia, Portugal.

[1] J.M.A. Frazão, J.M.C. Lourenço, M. Áurea Cunha, M.F. Laranjeira, J. Los and A.M.C. Moutinho, *J. Chem. Phys.* 104, 8393 (1996).

[2] L.F. Casinhas, J.M.A. Frazão, J.M.C. Lourenço, P. Limão Vieira, M. Áurea Cunha, M.L. Bhatt, J. Los and A.M.C. Moutinho, *XIX Int. Symp. On Molec. Beams, Rome* (2001).

## Publicado em:

*LIVRO DE RESUMOS  
DO 1º ENCONTRO  
NACIONAL DE FÍSICA  
ATÓMICA E  
MOLECULAR, 14, LIS-  
BOA, 13-14 ABRIL  
2004*

# ON-LINE OBJECT TRACKING WITH BAYESIAN NETWORKS

**Jorge, Pedro M.; Abrantes, Arnaldo J.;  
Marques, Jorge S.**

Departamento de Engenharia de Electrónica e Telecomunicações e  
de Computadores., ISEL, Lisboa, Portugal

A tracking system based on Bayesian networks was recently proposed. This system deals with difficult situations (e.g., occlusions, group formation and splitting) trying to recover the object identity provided it appears isolated again. This requires an off line processing of the video sequence which prevents its use in real time applications such as video surveillance. This paper describes a modified version of the BN tracker, tailored for on-line tracking of moving objects. This is achieved by gradually forgetting the influence of past information on the current decisions avoiding a combinatorial explosion and keeping the network complexity within reasonable bounds.

**Publicado em:**

*5th International  
Workshop on Image  
Analysis for  
Multimedia Interactive  
Services, Lisboa, APR  
2004*

# STACKED N-I-P-N-I-P HETEROJUNCTIONS FOR IMAGE RECOGNITION

**Vieira, M.; Fantoni, A.; Fernandes, M.; Louro, P.;  
Rodrigues, I.**

ISEL, Dept Elect & Telecommun Eng, P-1949014 Lisbon, Portugal

This work aims to clarify possible improvements and physical limits of the Color Laser Scanned Photodiode image sensor when used as high sensitive non-pixel image reader. A new design based on a stacked n-i-p-n-i-p heterojunction is proposed and compared with the old single n-i-p sensing structure. Results show that a B-W image is acquired with an improved resolution. The readout frequency is optimized showing that scans speeds up to 10(4) lines per second can be achieved without degradation in the resolution. A physical model is presented and supported by an electrical and a numerical simulation of the output characteristics of the sensor.

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AMORPHOUS AND  
NANOCRYSTALLINE  
SILICON-BASED FILMS-  
2003 762: 199-204,  
2003 MATERIALS  
RESEARCH SOCIETY  
SYMPOSIUM  
PROCEEDINGS  
Editor(s): Abelson JR,  
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H, Robertson J, Schiff  
EA IDS Number:  
BYo9N ISSN: 0272-  
9172

# LARGE AREA SINGLE AND STACKED P-I-N PHOTODIODES AS A COLOR IMAGE SENSORS

Louro, P.<sup>1</sup>; Fernandes, M.<sup>2</sup>; Fantoni, A.<sup>1</sup>;  
Macarico, A.<sup>1</sup>; Carvalho C.N. de<sup>2</sup>;  
Lavareda, G.<sup>2</sup>; Vieira, M.<sup>1</sup>

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<sup>2</sup> CFM-IST, Portugal

Single and stacked p-i-n sensing elements for image recognition and color extraction applications are presented. The aim of this work is to optimize the performance of the a-SiC:H thin films layers in order to enhance its performance when making part of the structure of large area image and colorsensors. The efforts are focused mainly on doped n- and p- type layers at high and low doping levels with and without carbon. The structural and optoelectronic properties of the single layers were determined through infrared and visible spectroscopy, temperature-dependent conductivity, and were complemented by CPM measurements. Junction properties, carrier transport, photogeneration and collection efficiency are investigated from dark and illuminated current-voltage characteristics and spectral response measurements, with and without additional background illumination and under different light bias conditions. The spectral response dependence on the applied voltage and on optical bias was also studied. Results show that the spectral sensitivity is strongly dependent on the applied voltage, namely the maximum spectral sensitivity shifts with the voltage, and at certain wavelengths the spectral response goes down to zero, which allows a different selectivity, and enables color recognition.

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SILICON CARBIDE  
2004-MATERIALS,  
PROCESSING AND  
DEVICES 815: 311-316,  
2004 MATERIALS  
RESEARCH SOCIETY  
SYMPOSIUM PRO-  
CEEDINGS, Editor(s):  
Dudley M, Gourma P,  
Kimoto T, Neudeck  
PG, Sadow SE  
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506 KEYSTONE DRIVE,  
WARRENDALE, PA  
15088-7563 USA IDS  
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# LARGE AREA P-I-N FLEXIBLE IMAGE SENSORS

**Vieira, M.<sup>1</sup>; Louro, P.<sup>1</sup>; Fernandes, M.<sup>1</sup>; Schwarz, R.<sup>2</sup>; Schubert, M.<sup>2</sup>**

- 1** ISEL, Elect Telecommun & Comp Dept, Lisbon, Portugal  
**2** Univ Stuttgart, Inst Phys Elekt, D-7000 Stuttgart, Germany

Large area p-i-n image sensors deposited on plastic substrates were produced at low temperatures (110degreesC) by PE-CVD and compared with similar sensors deposited on glass substrates. The same sensing element structure ZnO:Al/p(SiC:H)/i(Si:H)/n(SiC:H)/Al was used for both devices. In this work the efforts are focused mainly on the optimization of the output characteristics of the sensor when fabricated on plastic substrates. The role of the sensor configuration and readout parameters in the image acquisition process is analyzed. The optical-to-electrical transfer characteristics show a reasonable quantum efficiency under a red light pattern, broad spectral response, and reciprocity between light and image signal. First results show that the sensors deposited on flexible substrate present smaller light to dark sensitivity than those deposited on glass. In both, the non ohmic behavior of the transparent conductive oxide front contact blocks the carrier collection and leads to a surprising linear dependence of the image signal with the applied voltage.

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# TWO TERMINAL LARGE AREA SINGLE AND DOUBLE P-I-N DEVICES FOR IMAGE AND COLOR RECOGNITION

Louro, P.<sup>1</sup>; Vieira, M.<sup>1</sup>; Fantoni, A.<sup>1</sup>; Fernandes, M.<sup>1</sup>; Carvalho, C.N. de<sup>2</sup>; Lavareda, G.<sup>2</sup>

<sup>1</sup> ISEL, Elect Telecommun & Comp Dept, Lisbon, Portugal  
<sup>2</sup> CFM-IST, Portugal

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. All have the same intrinsic layer and in the doped layers the resistivity and optical gap was controlled through the addition of methane to the doping gas. The current-voltage characteristics and the spectral sensitivity under different illumination conditions are analyzed. The sensor output characteristics are evaluated under different read-out voltages and scanner wavelengths. To extract information on image range, 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.

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# A REAL-TIME OPTICAL SIGNAL AND IMAGE PROCESSING P-I-N/P-I-N DEVICE

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

ISEL, Elect Telecommun & Comp Dept, P-1949014 Lisbon, Portugal

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 AMORPHOUS AND  
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 MATERIALS RESEARCH  
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 Carius R, Biswas R  
 MATERIALS RESEARCH  
 SOCIETY, 506 KEY-  
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 RENDALE, PA 15088-  
 7563 USA IDS  
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Large area ( $4 \times 4 \text{ cm}^2$ ) optical signal and image processing (OSIP) devices were produced at low temperatures ( $110^\circ\text{C}$ ) by PE-CVD. The OSIP device consists of two stacked sensing/switching diodes ( $\text{p}(\text{SiC:H})/\text{i}(\text{Si:H})/\text{n}(\text{SiC:H})$ ) with or without an internal blocking layer between them and two semitransparent contacts. An optical scanner is used for charge readout. In this work the main emphasis will be put on the analysis of the optical characteristics. The use of a metal grid ( $290 \times 290 \text{ } \mu\text{m}^2$ ) Cr pixels with  $40 \text{ } \mu\text{m}$  spacing) between the two diodes, working as light screening layer or as floating anode via an a-SiN insulator layer, is analyzed. Its influence on the transfer functions, resolution, responsivity and response time of the sensor is presented. The various design parameters trade-offs are discussed. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between the optical and the electrical images. When the light screening floating anode is present an effective optical decoupling from both photodiodes is achieved while maintaining a good electrical conductivity and an increased light-to-dark sensitivity. A trade-off is established between sensor design and light pattern and scanner wavelengths in order to minimize the cross talk between the write and the read beams and to improve the light to dark sensitivity.

# MOVING TARGETS TRAJECTORY PARAMETERS ESTIMATION USING THE SIGNATURE CURVATURE INFORMATION

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Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

It is well known that a moving target induces a Doppler-shift and a Doppler-spread on the returned signal in the slow-time frequency domain. Most of the techniques proposed in recent literature take advantage of this knowledge to retrieve the moving target image and velocity parameters. The azimuth velocity of a moving target is the responsible for the spread in the slow-time frequency domain whereas the slant-range velocity induces the Doppler-shift. Given a PRF, the Doppler-shift,  $f_D$ , is confined to, where  $f_{D0}$  is the azimuth Doppler-shift induced by a moving target with slant-range velocity  $v$ , when the carrier wavelength is  $\lambda$ . If the signal is aliased (the induced Doppler-shift exceeds  $PRF/2$ ) it has been mostly accepted that the true moving target slant-range velocity cannot be uniquely determined using a single antenna and a single pulse scheduling. The traditional solution to resolve such targets consists in increasing the PRF, or alternatively, in using a non-uniform PRF as proposed recently. PRF increasing leads to a decrease in the maximum unambiguous range swath, besides the huge memory requirements to store the received signal. The use of a non-uniform PRF needs a non-conventional pulse scheduling. Moreover, non-uniform sampling introduces higher complexity in image reconstruction. Using typical SAR mission parameters, a single sensor, and uniform pulse scheduling, we readily conclude that the maximum unambiguous range velocity is usually very small. Herein we present a novel technique to estimate all the trajectory parameters of fast moving targets using a single SAR sensor without increasing the PRF. The basic reasoning is that, although the returned echoes may be aliased in the azimuth direction, its phase and amplitude are informative with respect to the moving target trajectory parameters. The proposed methodology samples the data in the spatial domain and tries to extract the data along the signature curve that is dependent of the moving target trajectory parameters. We start by writing the received signal, after pulse compression, in the spatial domain. We then write explicitly the moving target signature parameterized by the trajectory parameters. By assuming that the moving target signature is immersed in white noise we derive a maximum likelihood

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*Moving Targets Trajectory Parameters Estimation Using The Signature Curvature Information*, European Conference on Synthetic Aperture Radar, EUSAR 2004, Ulm, Alemanha, Maio de 2004.

estimator for the moving target trajectory parameters. At the end of the paper we present results using simulated and real data from the MSTAR public release data set.

# ON-LINE TRACKING GROUPS OF PEDESTRIANS WITH BAYESIAN NETWORKS

**Jorge, Pedro M.; Marques, Jorge S.; Abrantes, Arnaldo J.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

A video tracker should be able to track multiple objects in the presence of occlusions. This is a difficult task since there is not enough information during the occlusion time intervals. This paper proposes a tracking system which solves these difficulties, allowing a long term tracking of multiple interacting objects. First active regions are tracked using simple image analysis techniques. Then, a Bayesian network is used to label/recognize all the detected trajectories, taking into account the interaction among multiple objects. Experimental results are provided to assess the proposed algorithm with PETS video sequences.

**Publicado em:**

*6th IEEE International Workshop on Performance Evaluation of Tracking and Surveillance (PETS), Prague, Czech Republic, MAY 2004*

# MULTI-USER MIMO PERFORMANCE APPLIED TO UMTS HSDPA

**Vieira, P.<sup>1,2</sup>; Rodrigues, A.<sup>2</sup>**

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The aspects of applying MIMO techniques to the UMTS HSDPA transmission, in order to increase transmission rate in UTRAN are introduced. It is shown that Shannon capacity measure, working as the uplink transmitted channel metric, performs a major role on transmission rate determination, Frame Error Rate estimation, and scheduling at the Node B. A UMTS HSDPA simulator using MIMO techniques was developed. It allowed to estimate the MIMO capacity enhancement to the UMTS HSDPA system and to conclude that overall MIMO usage increases UMTS HSDPA system performance.

# OPTICAL SIGNAL AND IMAGE PROCESSING DEVICE OPTIMIZED FOR OPTICAL READOUT

**Vieira, M.; Fernandes, M.; Louro, P.; Mendes, C.; Schwarz, R.; Vigranenko, Y.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores, ISEL, Lisboa, Portugal

Large area ( $4 \times 4 \text{ cm}^2$ ) optical signal and image processing (OSIP) devices were produced at low temperatures by Plasma Enhanced Chemical Vapour Deposition (PE-CVD). The OSIP device consists of two stacked sensing/switching diodes ( $p(\text{SiC:H})/i(\text{Si:H})/n(\text{SiC:H})$ ) with an internal light blocking layer between them and two semitransparent contacts. An optical scanner is used for charge readout. In this work the main emphasis will be put on the analysis of the optical characteristics. The use of a metal grid ( $290 \times 290 \mu\text{m}^2$ ) Cr pixels with  $40 \mu\text{m}$  spacing) between the two diodes, working as light screening layer or as floating anode via an a-SiN insulator layer, is analyzed. Its influence on the transfer functions, resolution, responsivity and response time of the sensor is presented. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between the optical and the electrical images. When the light screening floating anode is present an effective optical decoupling from both photodiodes is achieved while maintaining a good electrical conductivity and an increased light-to-dark sensitivity. A trade-off is established between sensor design and light pattern and scanner wavelengths in order to minimize the cross talk between the write and the read beams and to improve the light to dark sensitivity. (c) 2004 Elsevier B.V. All rights reserved

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2005, Symposium of  
the European-  
Materials-Research-  
Society on Si-Based  
Photonics - Towards  
True Monolithic  
Integration, Strasbourg,  
FRANCE, MAY 25-28,  
2004, European Mat  
Res Soc

# THE PRESENTER ROLE IN A MULTI-AGENT ENVIRONMENT: A KNOWLEDGE SHARING APPROACH

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 Based Simulation  
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This paper focuses on agent-to-human presentation of the agent knowledge-level in a multi agent environment. The presentation competence is regarded as an agent's role - the presenter role. In our approach the design of the presenter role is driven by two main concerns: i) the sharing of knowledge via ontology commitment, and ii) the presenter's awareness of each exposed agent's role. The construction of this role comes across two inner issues: one is to properly present knowledge to the human user; the other is to cope with diverse knowledge-level representations. Our proposal addresses both issues from a communication based approach. We suggest that a standard semantic language (such as FIPA SL) should be used within each communicative act's content, and that modern and platform independent user-interface components (such as Java Swing) should be used to communicate with human users. To materialize this proposal, we adopted FIPA specifications and used JADE framework as base of the development process. Ontology specifications were conducted using the Protégé ontology editor.

# SIMULADOR DE RECEPTOR PARA SISTEMAS DE POSICIONAMENTO

**Sousa, Fernando M.G.**

Instituto Superior de Engenharia de Lisboa.

Aspectos do desenvolvimento de um simulador de receptor para os sistemas de posicionamento GPS modernizado e Galileo. Estrutura dos sinais dos sistemas de posicionamento. Arquitectura dos receptores “*software radio*”. Aquisição e seguimento. Arquitectura do simulador e extensões. Exemplos de simulação.

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*Expoinformática 2004,*  
*Maio 11-13, ISEL,*  
*Lisboa.*

# UNIFYING EMOTION AND COGNITION: THE FLOW MODEL APPROACH

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17th International  
Florida Artificial  
Intelligence Research  
Society Conference,  
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Growing experimental evidence shows the fundamental role that emotion plays in intelligent behaviour as well as the close relationship between emotion and what is classically known as cognition. Due to this evidence different models have been proposed to support emotion in artificial agents. However, the classical separation between emotion and cognition still prevails, not favouring the definition of a general framework to support the implementation of emotional agents. In this paper we present a model that unifies emotion and cognition as two symbiotically integrated aspects of intelligent behaviour. Despite being inspired by biological processes, the proposed model is independent of specific physiological or psychological details in order to support the implementation of concrete agents of different kinds and levels of complexity.

# OPTOELECTRONIC CHARACTERIZATION OF A-SIC : H STACKED DEVICES

**Louro, P.; Fantoni, A.; Fernandes, M.; Macarico, A.; Schwarz, R.; Vieira, M.**

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The aim of this work is the optoelectronic characterization of double p-i-n stacked devices based on a-Si alloy materials, in order to evaluate their suitability in large area optical sensors. Photogeneration, collection efficiency and carrier transport are investigated from dark and illuminated current-voltage characteristics and spectral response measurements, with and without additional background illumination and different electrical bias conditions. Results show that the collection efficiency depends on the device configuration and on the optical and electrical bias. The carrier collection is mainly dependent on the front and back intrinsic layers thickness and on the composition of the p-type doped layers. When wide band gap p-layers are used, the asymmetric distribution of the electrical field controls the transport mechanism. Under red optical bias the electrical field is enhanced at the front cell and decreased at the back one leading to an increased red light-to-dark sensitivity. A numerical simulation supports the discussion of the experimental results. Considerations about induced electric field and inversion layers at the interfaces and generation recombination process are used to explain the device output. (C) 2004 Elsevier B.V. All rights reserved.

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3093

# OPTICALLY ADDRESSED READ-WRITE DEVICE BASED ON TANDEM HETEROSTRUCTURE

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An optically addressed read-write sensor based on two stacked p-i-n heterojunctions is analyzed. The device is a two terminal image sensing structure. The charge packets are injected optically into the p-i-n writer and confined at the illuminated regions changing locally the electrical field profile across the p-i-n reader. An optical scanner is used for charge readout. The role of the sensor configuration and readout parameters on the image acquisition process is analyzed. The presence of a metallic light-screening layer between the writer and the reader proved to be effective to optically decouple the two p-i-n structures, while maintaining good electrical conductivity. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between light and image signal. A numerical simulation supports the imaging process.

# DEGRADATION OF PARTICLE DETECTORS BASED ON A-SI : H BY 1.5 MEV HE-4 AND 1 MEV PROTONS

Schwarz, R.<sup>1</sup>; Braz, T.<sup>1</sup>; Sanguino, P.<sup>1</sup>; Ferreira, P.<sup>1</sup>; Macarico, A.<sup>2</sup>; Vieira, M.<sup>2</sup>; Marques, C.<sup>3</sup>; Alves, E.<sup>3</sup>

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<sup>3</sup> ITN, P-2686953 Sacavem, Portugal

Photoconductivity as a measure of the majority carrier mobility-lifetime product is monitored in intrinsic amorphous silicon film (a-Si:H) when subjected to a 1.5 MeV He-4 beam. In a second step we looked at the changes of device performance in a 5 µm thick a-Si:H based detector structure which was subjected to a 1 MeV proton beam that assures a homogeneous damage profile. We find that the Rose coefficient increases to near unity after strong irradiation indicating the transition from bi- to monomolecular recombination. The p-i-n device shows changes that can be related to the properties of the thick intrinsic layer. As a by-product we can reconstruct the particle beam profile using the analytical fit to the fluence dependence of photosensitivity. (C) 2004 Elsevier B.V. All rights reserved.

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# OPTOELECTRONIC CHARACTERIZATION OF A-SIC:H STACKED DEVICES

**Louro, P.; Fantoni, A.; Fernandes, M.; Macarico, A.; Schwarz, R.; Vieira, M.**

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The aim of this work is the optoelectronic characterization of double p-i-n stacked devices based on a-Si alloy materials, in order to evaluate their suitability in large area optical sensors. Photogeneration, collection efficiency and carrier transport are investigated from dark and illuminated current-voltage characteristics and spectral response measurements, with and without additional background illumination and different electrical bias conditions. Results show that the collection efficiency depends on the device configuration and on the optical and electrical bias. The carrier collection is mainly dependent on the front and back intrinsic layers thickness and on the composition of the p-type doped layers. When wide band gap p-layers are used, the asymmetric distribution of the electrical field controls the transport mechanism. Under red optical bias the electrical field is enhanced at the front cell and decreased at the back one leading to an increased red light-to dark sensitivity. A numerical simulation supports the discussion of the experimental results. Considerations about induced electric field and inversion layers at the interfaces and generation-recombination process are used to explain the device output.

# OPTICALLY ADDRESSED READ–WRITE DEVICE BASED ON TANDEM HETEROSTRUCTURE

**Vieira, M.; Fernandes, M.; Fantoni, A.; Louro, P.; Schwarz, R.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

An optically addressed read–write sensor based on two stacked p–i–n heterojunctions is analyzed. The device is a two terminal image sensing structure. The charge packets are injected optically into the p–i–n writer and confined at the illuminated regions changing locally the electrical field profile across the p–i–n reader. An optical scanner is used for charge readout. The role of the sensor configuration and readout parameters on the image acquisition process is analyzed. The presence of a metallic light-screening layer between the writer and the reader proved to be effective to optically decouple the two p–i–n structures, while maintaining good electrical conductivity. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between light and image signal. A numerical simulation supports the imaging process.

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# CONSTANT ENERGY AND CLEAN SEGMENT SEQUENCES BASED ON MLS APPLIED TO ROOM IMPULSE RESPONSE MEASUREMENT

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- 1 Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal
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and Vibration, ICSV12,  
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Petersburg, Russia.*

Two new methods based in MLS technique referred as Constant Energy and Clean Segment Sequences are presented for applications where time limited high noise background levels occur. This technique consists in the isolation of the segments of appearance of the noise inside the MLS sequence for further signal processing. The choice of each technique depends on the SNR value for the identified noise segment. The Clean Segment is used for very low SNR values consisting in blanking the noise segment but keeping the same sequence period. The Constant Energy is used for reasonable low SNR values consisting in reducing the level of the noise segment keeping the same energy for the whole sequence.

Compared against the classic MLS approach, the increasing of the computational complexity of these techniques is irrelevant.

In order to compare the classic MLS approach against the Constant Energy and Clean Segment Sequences techniques, several examples are presented. The advantages and disadvantages of each technique are also discussed.

# THE ACTIAS SYSTEM: SUPERVISED MULTI-STRATEGY LEARNING PARADIGM USING CATEGORICAL LOGIC.

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- 1 Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal
- 2 Departamento de Informática, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

One of the most difficult problems in the development of intelligent systems is the construction of the underlying knowledge base. As a consequence, the rate of progress in the development of this type of system is directly related to the speed with which knowledge bases can be assembled, and on its quality. We attempt to solve the knowledge acquisition problem, for a Business Information System, developing a supervised multi-strategy learning paradigm. This paradigm is centred on a collaborative data mining strategy, where groups of experts collaborate using data-mining process on the supervised acquisition of new knowledge extracted from heterogeneous machine learning data models.

The Actias system is our approach to this paradigm. It is the result of applying the graphic logic based language of sketches to knowledge integration. The system is a data mining collaborative workplace, where the Information System knowledge base is an algebraic structure. It results from the integration of background knowledge with new insights extracted from data models, generated for specific data modelling tasks, and represented as rules using the sketches language.

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 ICKEDS'04:  
 International  
 Conference on  
 Knowledge Engineer  
 and Decision Support,  
 Porto, 2004*

# THE 5RINGS “TEAM DESCRIPTION PAPER”

**Silva, Paulo T.<sup>1</sup>; Araújo, Paulo<sup>1</sup>; Remédios, Afonso<sup>1</sup>; Lopes, Carlos<sup>1</sup>; Basílio, Bruno<sup>1</sup>; Loureiro, Tiago<sup>2</sup>; Moniz, Luís<sup>2</sup>; Coelho, Helder<sup>2</sup>**

**1** Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores, ISEL, Lisboa, Portugal

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In this paper we describe the approach of the 5RingsTeam to the complexity of the RoboCupRescue simulation environment. We consider two decisive contributors to that complexity: the communication scarceness and the multiplicity of tasks to be accomplished. We propose to approach the communication scarceness aspect by two different perspectives: (a) the leadership concept (both static and emergent); and (b) the information sharing at different aggregation levels. We adopted a two level's stratification of the multiplicity of tasks to be accomplished: (a) the agent (personal) level; and (b) the team (social) level. At the present stage of development, our framework supports the search and rescue of endangered civilians (ambulance team); the repair of blocked routes to refugees (police force); and the extinguishing of fires (fire brigade). The centers (police office, ambulance center and fire station) act mainly as resource dispatchers as they call for resources (e.g. a police force), in accordance to the indications received from other agents (e.g. a blockaded ambulance team) without the required skills to handle a perceived situation (e.g. a road blockade).

**Publicado em:**

*RoboCup2004  
Symposium. July 4-5,  
Lisbon, Portugal*

# INDOOR PROPAGATION MODELS AND RADIO PLANNING FOR WLANS

**Lopes, R.; Freixo, P.; Serrador, A.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

WLANS are nowadays at the top of the mass market networks technologies. They are essentially implemented indoors, where the traditional planning tools are not yet focused. Although the concerning to improve the radio planning quality, the existing propagation models can still be sharpened for better outcomes, mainly in large buildings. A new propagation model is proposed and evaluated with measurements at 2.4GHz and also a planning tool is presented, with the ability to execute coverage and capacity analysis on indoor multi-floors environments. This model adapts itself to multiple indoor scenarios following the performed measurements.

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*1st International  
Conference on  
E-Business and  
Telecommunications  
Networks, Agosto,  
2004.*

# CONCEPTS OF SIMULTANEOUS USE IN THE CONVERGENCE OF WIRELESS SYSTEMS

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In the wireless communications future, users will claim availability of services, neglecting the underlined systems in use. Users simply aim to be Always Best Connected (ABC). To satisfy this need, integration and interworking are key aspects, leading to simultaneous use concepts of services, systems and operators. Eleven concepts of simultaneous use are identified and analysed. Despite several identified cons, these concepts present overcoming pros, leading to a promising future of integration of wireless.

**Publicado em:**

*The 13th IST Mobile &  
Wireless  
Communications 2004.*

# THE MEAN SHIFT AND THE UNIFIED FRAMEWORK

**Abrantes, Arnaldo J.; Marques, Jorge S.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

This paper considers two classes of algorithms for the representation of data points using centroids: the unified framework and the mean shift algorithm. The relationship between both approaches is presented showing that the mean shift algorithm fits within the unified framework being equivalent to snake with Cohen potential. However it does not use competitive learning as the other methods considered in the unified framework. The advantages of both types of techniques are exemplified through examples.

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*17th International  
Conference on Pattern  
Recognition (ICPR),  
Cambridge, UK, (1)  
244-247, AUG 2004*

# ESTIMATION OF THE BAYESIAN NETWORK ARCHITECTURE FOR OBJECT TRACKING IN VIDEO SEQUENCES

**Jorge, Pedro M.; Abrantes, Arnaldo J.; Marques, Jorge S.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

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Cambridge, UK, (2)  
732-735, AUG 2004*

It was recently proposed the use of Bayesian networks for object tracking. Bayesian networks allow to model the interaction among detected trajectories, in order to obtain a reliable object identification in the presence of occlusions. However, the architecture of the Bayesian network has been defined using simple heuristic rules which fail in many cases. This paper addresses the above problem and presents a new method to estimate the network architecture from the video sequences using supervised learning techniques. Experimental results are presented showing that significant performance gains (increase of accuracy and decrease of complexity) are achieved by the proposed methods.

# A-SIC: H/A-SI: H TANDEM PHOTODIODES: A NUMERICAL SIMULATION

**Fantoni, A.; Fernandes, M.; Louro, P.;  
Rodrigues, I.; Vieira, M.**

Departamento de Engenharia de Electrónica e Telecomunicações e  
de Computadores., ISEL, Lisboa, Portugal

It is well known from the literature that, in order to optimize the light power conversion, the geometry of the cell and the thickness of the absorber layers must be adjusted to the light absorption profile. If there is a mismatch between the electron-hole pairs generated in the sub-cells, the total collected current is limited by the sub-cell absorbing the lowest number of photons. We have found the photocurrent profile in these conditions to be dependent on the light absorption profile, that is, on the incident light wavelength and intensity. Our experiments and analysis reveal the photocurrent profile to have a strong nonlinear dependence on the externally applied bias in the range around the open circuit value, indicating the superposition of different, concurring effects that lead the photocurrent to alternatively increase and decrease before finally entering in its secondary state. The possibility of relating such behavior to the light intensity and color, leaves an open discussion on the possibility of using these structures and this effect for color recognition sensors.

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*SENSORS AND ACTUA-  
TORS A PHYSICAL 113  
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2004*

# FOCUSING REASONING THROUGH EMOTIONAL MECHANISMS

**Morgado, L.; Gaspar, G.**

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Artificial Intelligence,  
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In concrete environments, where uncertainty and dynamism are pervasive and time and resources are limited, reasoning and decision-making processes raise important problems related both to adaptive ability and to the computational complexity of the underlying cognitive mechanisms. In this paper we propose that a symbiotic integration between emotion and cognition is a key aspect to address these problems. To concretize this view we present an agent model where emotion and cognition are modelled as two integrated aspects of intelligent behaviour and where affective-emotional mechanisms are used to support adaptability and to focus the reasoning and deliberation mechanisms to cope with their computational complexity.

# A-SIC: H/A-SI: H TANDEM PHOTODIODES: A NUMERICAL SIMULATION

**Fantoni, A.; Fernandes, M.; Louro, P.;  
Rodrigues, I.; Vieira, M.**

DEETC, ISEL, P-1949014 Lisbon, Portugal

It is well known from the literature that, in order to optimize the light power conversion, the geometry of the cell and the thickness of the absorber layers must be adjusted to the light absorption profile. If there is a mismatch between the electron-hole pairs generated in the sub-cells, the total collected current is limited by the sub-cell absorbing the lowest number of photons. We have found the photocurrent profile in these conditions to be dependent on the light absorption profile, that is, on the incident light wavelength and intensity. Our experiments and analysis reveal the photocurrent profile to have a strong nonlinear dependence on the externally applied bias in the range around the open circuit value, indicating the superposition of different, concurring effects that lead the photocurrent to alternatively increase and decrease before finally entering in its secondary state. The possibility of relating such behavior to the light intensity and color, leaves an open discussion on the possibility of using these structures and this effect for color recognition sensors. (C) 2004 Elsevier B.V. All rights reserved.

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SCIENCE SA, PO BOX  
564, 1001 LAUSANNE,  
SWITZERLAND IDS  
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0924-4247*

# A DYNAMIC SYSTEM-LEVEL SIMULATION TOOL FOR UMTS FDD

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This paper presents a tool for dynamic simulation of radio resources in UMTS FDD. The developed tool provides an integrated environment for users scenario definition, environment edition, base stations planning, simulation and analysis. This tool can also be used to evaluate the impact of new services, different system settings or new subscriber profiles, in the system's global performance. For implementing the different mechanisms of WCDMA radio technology, the simulation tool kernel was supported by a system-level, dynamic, stochastic and event driven simulation model. Both uplink and downlink directions are considered, including soft handover connections. The final results confirm the developed tool validity and its good functionality in relation to simulation scenario definition, simulation and analysis phases.

**Publicado em:**

*ICETE'2004  
- International  
Conference on E  
Business and  
Telecommunication  
Networks, Aug, 2004*

# ADJACENT CHANNEL INTERFERENCE - IMPACT ON THE CAPACITY OF WCDMA/FDD NETWORKS

**Figueiredo, Daniel; Matos, Pedro; Cota, Nuno;  
Rodrigues, António**

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The adjacent channel interference (ACI) can result in a reduced network capacity in a multioperator WCDMA/FDD environment. This paper is devoted to the study of the ACI, using a static simulator. Simulations were performed in order to identify particular scenarios and network compositions where ACI plays a major role in the system capacity. On the basis of the results, the authors identify the best strategy for frequency deployment within the available spectrum. It is demonstrated that the macro carrier should be located in the centre of the frequency band, protected from the ACI introduced by other operators. It is, in fact, the carrier which suffers the greatest losses caused by the increase in ACI. Furthermore, the micro carrier should be placed as close as possible to the adjacent channel of other operators in order to maximize system capacity.

**Publicado em:**

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International  
Conference on E  
Business and  
Telecommunication  
Networks, Aug, 2004*

# LARGE AREA IMAGE SENSING STRUCTURES BASED ON A-SIC : H: A DYNAMIC CHARACTERIZATION

**Fernandes, M.<sup>1</sup>; Vieira, M.<sup>1</sup>; Rodrigues, I.<sup>1</sup>; Martins, R.<sup>2</sup>**

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**2** Univ Nova Lisboa, Fac Ciencias & Tecnol, Dept Mat Sci, P-2825 Monte De Caparica, Portugal

In recent works large area hydrogenated amorphous silicon p-i-n structures with low conductivity doped layers were proposed as single element image sensors. The working principle of this type of sensor is based on the modulation, by the local illumination conditions, of the photocurrent generated by a light beam scanning the active area of the device. In order to evaluate the sensor capabilities is necessary to perform a response time characterization. This work focuses on the transient response of such sensor and on the influence of the carbon contents of the doped layers. In order to evaluate the response time a set of devices with different percentage of carbon incorporation in the doped layers is analyzed by measuring the scanner-induced photocurrent under different bias conditions. (C) 2004 Elsevier B.V. All rights reserved.

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# PERFORMANCE OF ENHANCED-UMTS HSDPA USING TRANSMIT DIVERSITY AND POWER CONTROL SCHEMES

**Silva, João Carlos; Souto, Nuno;  
Rodrigues, António**

Departamento de Engenharia de Electrónica e Telecomunicações e  
de Computadores., ISEL, Lisboa, Portugal

This paper addresses the performance of the downlink High Speed Data Packet Access (HSDPA) in QPSK mode. Transmit Diversity (TD) enhancement schemes such as Space Time Transmit Diversity (STTD) and Selective Transmit Diversity (STD), alongside a Power Control (PC) scheme, are covered to improve the system capacity. To evaluate the performance and the advantages of all the schemes under different conditions, several combinations of these were simulated in the AWGN, Indoor A and Pedestrian A channels. For the best combination, a gain of 11.5dB can be achieved, for a BLER of 1%.

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*WPMC'2004 -  
International  
Symposium on  
Wireless Personal  
Multimedia  
Communications, Sep,  
2004*

# A DYNAMIC SIMULATION OF PACKET SWITCHED DATA OVER UMTS FDD

**Cota, Nuno; Rodrigues, António**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

A dynamic and system-level simulation tool for performance evaluation of packet switched data services in UMTS FDD is presented on this paper. The simulator provides an efficient and flexible interface, with an integrated framework for complete scenario definition, simulation and results analysis.

Simulation considers subscriber's profile mobility behavior on a urban environment and radio resource demand characterization to evaluate the impact of new services introduction on a WCDMA access network. Both downlink and uplink direction are considered, including several soft handover connections. Thus, a stochastic and event driven simulation model with a process oriented approach is implemented on a C++ programming language, providing a user friendly Windows interface.

**Publicado em:**

*WPMC'2004  
- International  
Symposium on  
Wireless Personal  
Multimedia  
Communications, Sep,  
2004*

# INNOVATIONS-BASED CODE DISCRIMINATOR FOR GPS/GALILEO BOC SIGNALS

Nunes, Fernando D.<sup>1</sup>; Sousa, Fernando M.G.<sup>2</sup>;  
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Binary offset carrier (BOC) modulation was considered for modernized military GPS and for the European Navigation System Galileo. Although it performs better than the conventional BPSK modulation, the BOC waveforms have autocorrelation functions with multiple peaks that lead to potential tracking ambiguities. In the paper we propose to minimize this problem with a bank of extended Kalman filters (EKF) that track the phase/frequency from the quadrature components of the incoming signal. The code discriminator is a weighted sum of code delays with the weights being nonlinear functions of the EKF innovations. When compared to the early\_late power discriminator the proposed algorithm is much less prone to lose tracking of the BOC autocorrelation main peak.

**Publicado em:**

*Proceedings of the  
IEEE Vehicular  
Technology Conference  
2004-Fall, "Wireless  
Technologies for  
Global Security,"  
September 26-29,  
Los Angeles, CA*

# INTEROPERABILITY AMONG ITS SYSTEMS WITH ITS-IBUS FRAMEWORK

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Araújo, P.<sup>1</sup>; Abrantes, A.<sup>1</sup>; Jorge, P.<sup>1</sup>;  
Gomes, J. Sales<sup>2</sup>; Jacquet G.<sup>2</sup>; Amador, A.<sup>2</sup>**

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*“Solutions for Future  
 Manufacturing  
 Systems”, Published  
 by Springer, SEP,  
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 pages 241-250,  
 em 2004*

This paper presents and discusses the extended Via-Verde business model from the point of view of the underlying requirements for the virtual business processes. The extension of Via-Verde concept to other services beyond the motorway toll collection has increased the number of independent companies involved. The complex networked scenario resulted on a proposal of an intelligent transport system – interoperability bus (ITS-IBus) (Gomes et. al. 2003) (Osorio, et. al. 2003-a) aiming to promote a generalized interoperability among heterogeneous (multi-vendor) technological subsystems. The ITS-IBus initiative has been developing since then, a reference implementation of a peer-to-peer service based framework with pluggable feature and a set of common agreed interfaces for coupling different technological systems. An important objective is to increase the quality of the offered services by establishing a flexible execution and coordination framework for the collaborative distributed business processes.

# AN INNOVATIONS APPROACH TO FALSE-LOCK MITIGATION FOR GPS/GALILEO BOC SIGNALS

Nunes, Fernando D.<sup>1</sup>; Sousa, Fernando M.G.<sup>2</sup>;  
Leitão, José M.N.<sup>1</sup>

<sup>1</sup> Instituto de Telecomunicações / Instituto Superior Técnico

<sup>2</sup> Instituto Superior de Engenharia de Lisboa.

Binary offset carrier (BOC) modulation was considered for modernized military GPS and for the European Navigation System Galileo. Although it performs better than the conventional BPSK modulation, the BOC waveforms have autocorrelation functions with multiple peaks that lead to potential tracking ambiguities. To mitigate this problem we propose an architecture where the conventional structure (PLL+DLL) is replaced with a bank of stochastic nonlinear filters that estimate the incoming carrier phase, frequency and frequency-rate (modeled as the components of a state vector). The code discriminator is a weighted sum of code delays with the weights being nonlinear functions of the filters innovations.

Two solutions are proposed and compared for the state vector estimation. When compared to the early-late power discriminator the proposed algorithms are much less prone to lose tracking of the BOC autocorrelation main peak while allowing the receiver to cope with a broader range of code delay errors. Besides, the resulting receiver provides information about the emitter/receiver trajectory dynamics (through the state vector estimates) and the quality of the received signals (through the innovations processes).

**Publicado em:**

*Proceedings of the  
ION GNSS 2004, pp.  
2636-2644, September  
21-24, Long Beach, CA*

# A NON-PIXEL IMAGE READER FOR CONTINUOUS IMAGE DETECTION BASED ON TANDEM HETEROSTRUCTURES

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

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*SENSORS AND ACTUATORS A PHYSICAL* 115  
(2-3): 191-195, SEP 21  
2004

An optically addressed read-write sensor based on two stacked p-i-n heterojunctions is analyzed. The device is a two terminal image sensing structure. The charge packets are injected optically into the p-i-n writer and confined at the illuminated regions changing locally the electrical field profile across the p-i-n reader. An optical scanner is used for charge readout. The design allows a continuous readout without the need for pixel-level patterning.

The role of light pattern and scanner wavelengths on the readout parameters is analyzed. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between light and image signal. A numerical simulation supports the imaging process. A black and white image is acquired with a resolution around 20  $\mu\text{m}$  showing the potentiality of these devices for imaging applications.

# OPTICAL CONFINEMENT AND COLOUR SEPARATION IN A DOUBLE COLOUR LASER SCANNED PHOTODIODE (D/CLSP)

**Vieira, M.; Fernandes, M.; Louro, P.; Fantoni, A.; Rodrigues, I.**

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

Large area n-i-p-n-i-p a-SiC:H heterostructures are used as sensing element in a double colour laser scanned photodiode image sensor (D/CLSP). This work aims to clarify possible improvements, physical limits and performance of CLSP image sensor when used as non-pixel image reader. Here, the image capture device and the scanning reader are optimized and the effects of the sensor structure on the output characteristics discussed. The role of the design of the sensing element, the doped layer composition and thickness, the read-out parameters (applied voltage and scanner frequency) on the image acquisition and the colour detection process are analysed. A physical model is presented and supported by a numerical simulation of the output characteristics of the sensor.

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*SENSORS AND ACTUATORS A PHYSICAL* 114  
(2-3): 219-223, SEP 21  
2004

# A NON-PIXEL IMAGE READER FOR CONTINUOUS IMAGE DETECTION BASED ON TANDEM HETEROSTRUCTURES

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 2004 ELSEVIER  
 SCIENCE SA, PO BOX  
 564, 1001 LAUSANNE,  
 SWITZERLAND, IDS  
 Number: 857TP ISSN:  
 0924-4247

An optically addressed read-write sensor based on two stacked p-i-n heterojunctions is analyzed. The device is a two terminal image sensing structure. The charge packets are injected optically into the p-i-n writer and confined at the illuminated regions changing locally the electrical field profile across the p-i-n reader. An optical scanner is used for charge readout. The design allows a continuous readout without the need for pixel-level patterning.

The role of light pattern and scanner wavelengths on the readout parameters is analyzed. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, and reciprocity between light and image signal. A numerical simulation supports the imaging process. A black and white image is acquired with a resolution around 20  $\mu\text{m}$  showing the potentiality of these devices for imaging applications. (C) 2004 Elsevier B.V. All rights reserved.

# NOVEL STRUCTURE FOR LARGE AREA IMAGE SENSING

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This work presents preliminary results in the study of a novel structure for a laser scanned photodiode (LSP) type of image sensor. In order to increase the signal output, a stacked p-i-n-p-i-n structure with an intermediate light-blocking layer is used. The image and the scanning beam are incident through opposite sides of the sensor and their absorption is kept in separate junctions by an intermediate light-blocking layer. As in the usual LSP structure the scanning beam-induced photocurrent is dependent on the local illumination conditions of the image. The main difference between the two structures arises from the fact that in this new structure the image and the scanner have different optical paths leading to an increase in the photocurrent when the scanning beam is incident on a region illuminated on the image side of the sensor, while a decreasing in the photocurrent was observed in the single junction LSP. The results show that the structure can be successfully used as an image sensor even though some optimization is needed to enhance the performance of the device. (C) 2004 Elsevier B.V. All rights reserved.

**Publicado em:**

*SENSORS AND ACTUATORS A-PHYSICAL 115 (2-3): 357-361, SEP 21 2004 ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND IDS Number: 857TP ISSN: 0924-4247*

# OPTICAL CONFINEMENT AND COLOUR SEPARATION IN A DOUBLE COLOUR LASER SCANNED PHOTODIODE (D/CLSP)

**Vieira, M.; Fernandes, M.; Louro, P.; Fantoni, A.; Rodrigues, I.**

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*SENSORS AND ACTUATORS A-PHYSICAL* 114  
 (2-3): 219-223,  
 SEP 1 2004  
 IEEE; *Elect Devices Soc ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND*  
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 851SE ISSN:  
 0924-4247

Large area n-i-p-n-i-p a-SiC:H heterostructures are used as sensing element in a double colour laser scanned photodiode image sensor (D/CLSP). This work aims to clarify possible improvements, physical limits and performance of CLSP image sensor when used as non-pixel image reader. Here, the image capture device and the scanning reader are optimized and the effects of the sensor structure on the output characteristics discussed. The role of the design of the sensing element, the doped layer composition and thickness, the read-out parameters (applied voltage and scanner frequency) on the image acquisition and the colour detection process are analysed. A physical model is presented and supported by a numerical simulation of the output characteristics of the sensor. (C) 2004 Elsevier B.V. All rights reserved.

# TOWARDS UBIQUITOUS TASK MANAGEMENT

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In the near future people will be surrounded by intelligent devices embedded in everyday objects where the knowledge and understanding of device attributes and capabilities will be a key enabler.

This paper describes the current state of our research in design distributed knowledge based devices as a solution to adapt spoken dialogue systems within ambient intelligence. In this context a spoken dialogue system is a computational entity that enables universal access to ambient intelligence for anyone, anywhere, at anytime. Allowing the use of any device through any media. Our aim is to build knowledge-based devices to enable its dynamic adaptation when integrated in dialogue systems. An example focused on household appliances is depicted.

**Publicado em:**  
*INTERSPEECH 2004,*  
*Jeju Coreia, OUT 8*  
*2004*

# MULTIPATH MITIGATION TECHNIQUE FOR BOC SIGNALS USING GATING FUNCTIONS

**Nunes, Fernando D.<sup>1</sup>; Sousa, Fernando, M.G.<sup>2</sup>; Leitão, José M.N.<sup>1</sup>**

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A new multipath mitigation technique is proposed for binary carrier offset (BOC) signals using the concept of gating function originally conceived for GPS C/A. The structure of the code loop for BOC signals is quite simple including only four real correlators. The results show that this method efficiently eliminates the ranging errors in the medium and long-delay regions, thus comparing favorably with conventional correlation techniques.

**Publicado em:**

*Proceedings of the 2nd European Space Agency Workshop on Satellite Navigation User Equipment Technologies (NAVITEC 2004), pp. 424-431, December 8-10, Noordwijk, The Netherlands.*

# AN ACQUISITION ALGORITHM FOR WEAK SIGNALS IN GALILEO AND MODERNIZED GPS SYSTEMS

Sousa, Fernando M.G.<sup>1</sup>; Nunes, Fernando D.<sup>2</sup>;  
Leitão, José M.N.<sup>2</sup>

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In the Galileo system, as in the modernized civil GPS, there are two-channel navigation signals including a *data channel*, carrying navigation data, and a *pilot channel*. This work addresses the problem of cold acquisition of weak two-channel navigation signals in a software receiver. Different approaches, with and without channels combination, and with coherent and non-coherent combination of primary code integrations, are analyzed, simulated and compared with alternative solutions.

**Publicado em:**

*Proceedings of the 2nd European Space Agency Workshop on Satellite Navigation User Equipment Technologies (NAVITEC 2004), pp. 480-487, December 8-10, Noordwijk, The Netherlands.*

# SIGNAL GENERATOR AND RECEIVER TOOLBOX FOR GALILEO/GPS SIGNALS

**Nunes, A.<sup>1</sup>; Ferreira, T.<sup>2</sup>; Borràs, J.<sup>3</sup>; Nunes, F.<sup>2,3</sup>; Sousa, F.<sup>2,4</sup>; Seco, G.<sup>5</sup>**

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 2nd European Space  
 Agency Workshop on  
 Satellite Navigation  
 User Equipment  
 Technologies (NAVITEC  
 2004), pp. 142-148,  
 December 8-10,  
 Noordwijk, The  
 Netherlands.*

Galileo is the European navigation system that will be part of the Global Navigation Satellite System (GNSS), designed for civilian needs, opened to international cooperation and operated commercially, that aims at offering satellite positioning services with guaranteed reliability. Receivers capable of taking full advantage of the new signals in an efficient way will have to be developed in the near future. Actually, some developments have started already. The design of those receivers will progress in parallel with the development of the Galileo system itself, as only with appropriate receivers it will be possible to fully exploit, test and validate the Galileo signals.

The main objective of project DNURS – Development of a Navigation Users Receiver Simulator – is to develop and validate a software receiver simulator tool for Galileo and GPS navigation signals. Rather than focusing on the radio frequency front-end or the navigation subsystems, emphasis is placed on the signal processing component of the receiver, i.e., the subsystems that process the incoming intermediate frequency or base-band samples and provide bit values, pseudo-ranges and carrier phase measurements.

The resulting alpha-version Software Receiver is an open, flexible, easily configurable, upgradeable, extensible, sample-wise, and user-friendly tool box. This tool box is complemented by a software signal generator and a considerable amount of models and configurable parameters (e.g. concerning acquisition, filter types), allowing the investigation of the new GPS and Galileo signals as well as their performance assessment. Issues such as interference mitigation modelling, acquisition techniques, multipath mitigation and performance comparison between various signals are only a few examples of how this tool can be used.

# TUNING THE SPECTRAL DISTRIBUTION OF P–I–N A-SiC:H DEVICES FOR COLOUR DETECTION

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

Departamento de Engenharia de Electrónica e Telecomunicações e de Computadores., ISEL, Lisboa, Portugal

ZnO:Al/p (SiC:H)/i (Si:H)/n (SiC:H) large area image and colour sensor are analysed. Carrier transport and collection efficiency are investigated from dark and illuminated current–voltage (I–V) dependence and spectral response measurements under different optical and electrical bias conditions. Results show that the carrier collection depends on the optical bias and on the applied voltage. By changing the electrical bias around the open circuit voltage it is possible to filter the absorption at a given wavelength and so to tune the spectral sensitivity of the device. Transport and optical modelling give insight into the internal physical process and explain the bias control of the spectral response and the image and colour sensing properties of the devices.

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*SENSORS AND ACTUATORS A PHYSICAL*  
available on line 23  
December 2004,  
in press



# ENGENHARIA MECÂNICA

Anuário Científico 2004

ISEL



# A FUZZY INTEGRATED APPROACH TO IMPEDANCE CONTROL OF ROBOT MANIPULATORS

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## Abstract

This paper presents an integrated fuzzy approach to recover the performance in impedance control, reducing the errors in position and force, considering uncertainties in the parameters of the manipulator dynamic model and contact surface or environment model. This integrated strategy considers a fuzzy adaptive compensator in the outer control loop that adjusts the manipulator tip position to compensate for uncertainties present in the environment. In the inner loop, a fuzzy sliding mode-based impedance controller compensates for uncertainties in the model of the manipulator, based on an inverse dynamics control law. The system error, defines the sliding surfaces of the fuzzy sliding controller as the difference between the desired and actual impedances. In order to evaluate the force/position tracking performance and to validate the proposed control structure, simulations results are presented with a three-degree-of freedom (3-DOF) PUMA robot manipulator.

## Publicado em:

*Livro de Resumos de  
1th ICINCO 2004 -  
International  
Conference in Control,  
Automation and  
Robotics, Escola  
Superior de  
Tecnologia, Instituto  
Politécnico de Setúbal,  
25-28 of August 23-  
27, Portugal*

# AN ASSESSMENT METHODOLOGY FOR E-BUSINESS AND E-COMMERCE IN THE AEC SECTOR

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- 1** Associate Professor Instituto Superior de Engenharia de Lisboa
- 2** Assistant Professors at Faculdade Ciências e Tecnologia da Universidade Nova de Lisboa, Senior Resercheres in UNINOVA

**ABSTRACT:** Recent studies have illustrated that the AEC sector has embraced e-Commerce and e-Business. Indeed, case studies demonstrate that the use of electronic collaborative and commerce platforms by the different players in the AEC sector can be as sophisticated as the best practices found in Automotive, Aeronautics or Retailing sectors. However, the same studies do also recog-nize that though the best practices are at the same level, they are much less frequently deployed. This paper presents a methodology based on business factors to assess the readiness and likeli-ness of the development of e-Business and e-Commerce between the disparate players in AEC projects.

# CAPACITANCE AND PHOTOELECTROCHEMICAL STUDIES FOR THE ASSESSMENT OF ANODIC OXIDE FILMS ON ALUMINIUM

Fernandes, J.C.S.<sup>1</sup>; Picciochi, R.<sup>1</sup>;  
Belo, M. da Cunha<sup>1</sup>; Moura e Silva, T.<sup>2</sup>;  
Ferreira, M.G.S.<sup>1,3</sup>; Fonseca, I.T.E.<sup>4</sup>

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## Abstract

Photoelectrochemical spectroscopy and capacitance measurements were used in this work to assess the electronic properties of the oxide films formed on 99.5% aluminium and 2024 T3 aluminium alloy by anodising in a sulphuric-boric bath. The morphology of these films was also studied by transmission electron microscopy cross-section observations. The results obtained indicate that the oxide films formed on aluminium show a n-type semiconductive behaviour, with bandgap energies that are identical for the oxides studied, despite their different characteristics. It was found out that capacitance measurements may be used as a valuable technique for the assessment of the quality of anodised layers, allowing the distinction between an efficient and an inefficient sealing. Therefore, they may be used to predict the corrosion resistance of these materials.

## Publicado em:

*Electrochimica Acta*,  
49 (2004) 4701-7407

# ESTUDOS DE FOTOELECTROQUÍMICA E CAPACIDADE EM FILMES DE ÓXIDO DE ALUMÍNIO

Picciochi, R.<sup>1</sup>; Fernandes, J.C.S.<sup>1</sup>;  
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Sociedade  
Iberoamericana de  
Electroquímica,  
S. José, Costa  
Rica (9-14 Fevereiro  
2004)*

Apesar de a alumina ( $\text{Al}_2\text{O}_3$ ) ser normalmente referida na literatura como isolante, com uma energia de banda proibida variando entre 8 e 9 eV [1], estudos recentes dos filmes de óxido formados sobre alumínio parecem indicar que estes óxidos apresentam propriedades semicondutoras do tipo n, exibindo transições ópticas para energias na gama 2.8 a 4.5 eV. A relação entre as propriedades de estado sólido dos filmes de óxido de alumínio e a sua resistência à corrosão tem sido objecto de várias interpretações [2-4]. Neste contexto, a espectroscopia fotoelectroquímica e as medidas de capacidade (abordagem de Mott-Schottky) foram usadas neste trabalho para caracterizar as propriedades electrónicas dos filmes de óxido formados, sob diferentes condições, em alumínio comercial (99.5%) e na liga de alumínio 2024-T3. Os resultados confirmam o carácter semicondutor destes filmes, que apresentam valores muito semelhantes de energia da banda proibida, apesar das suas diferentes características. Conclui-se ainda que as medidas de capacidade podem ser usadas na avaliação da qualidade dos filmes anódicos, permitindo a distinção entre um processo de colmatagem eficiente e um ineficiente. Desta forma, as medidas de capacidade poderão ser usadas na previsão da resistência à corrosão destes materiais.

# FLEXÃO DE ELEMENTOS CURVOS EM COMPÓSITOS OBTIDOS POR AUTOCLAVE

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Instituto Superior de Engenharia de Lisboa  
Departamento de Engenharia Mecânica – Secção de Projecto  
Mecânico

Com este trabalho pretende-se dar continuidade a um estudo analítico e numérico sobre o comportamento mecânico de vigas à flexão, contendo elementos curvos. Analisou-se a influência de duas sequências de empilhamento: simétrica e não simétrica. Estes elementos serão obtidos recorrendo ao processo de autoclave, usando pré-impregnados de fibras de vidro em matriz epoxídica, correntemente usados na produção de equipamento móvel. A simulação analítica foi feita com base na teoria multicamada de Ko e Jackson. Na simulação numérica foram implementados, no programa comercial ANSYS 8.0, modelos usando elementos de casca e sólidos, ambos de multicamada.

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*MÉTODOS  
COMPUTACIONAIS EM  
ENGENHARIA  
Lisboa, 31 de Maio –  
2 de Junho, 2004  
© APMTAC, Portugal  
2004*

# LINEAR-WAVELET NETWORKS

**Galvão, Roberto K.H.<sup>1</sup>; Becerra, Victor M.<sup>2</sup>;  
Silva, P.M.<sup>3</sup>; Calado, J.M.F.<sup>3</sup>**

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*International Journal of  
Applied Mathematics  
and Computer Science,*  
2004, Vol.14, No. 2,  
221-232.

This paper proposes a nonlinear regression structure comprising a wavelet network and a linear term. The introduction of linear term is aimed at providing a more parsimonious interpolation in high-dimensional spaces when the modelling samples are sparse. A constructive procedure for building such structures, termed linear-wavelet networks, is described. For illustration, the proposed procedure is employed in the frame dynamic system identification. In an example involving a simulated fermentation process, it is shown that a linear-wavelet network yields a smaller approximation error when compared with a wavelet network with the same number of regressions. The proposed technique is also applied to the identification of a pressure plant from experimental data. In this case, the results show that the introduction of wavelets considerably improves the prediction ability of a linear model. Standard errors on the estimated model coefficients are also calculated to the numerical conditioning of the identification process.

# REMOTE VIRTUAL LAB – A CONTROL SYSTEMS APPROACH

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Departamento de Engenharia Mecânica, ISEL, Lisboa, Portugal

In this paper is proposed an architecture to develop virtual control systems laboratories and put them available through the Internet. Such a virtual lab has been coupled with a remote real lab already reported. The remote accessed computational platform developed has been used by students of a control systems course lectured at the Mechanical Engineering Department of ISEL. Students' opinions on using that computational system are also presented in the current paper. Furthermore, the system has been design and implemented not only with teaching purposes but also aiming to achieve a framework that could help control systems engineers on their professional activities. Copyright © 2004 IFAC

**Publicado em:**

*Livro de Abstracts da IBCE' 2004, IFAC Workshop in Internet Based Control Education, Grenoble, França, Setembro de 2004.*

# STUDIES ON SULPHURIC-BORIC ACID ANODISING PROCESSES FOR ALUMINIUM AND 2024 ALUMINIUM ALLOY

**Fernandes, J.C.S.<sup>1</sup>; Picciochi, R.<sup>1</sup>;  
Belo, M. da Cunha<sup>1</sup>; Moura e Silva, T.<sup>2</sup>;  
Ferreira, M.G.S.<sup>1,3</sup>; Fonseca, I.T.E.<sup>4</sup>**

- 1 IST, Department of Chemical Engineering, Lisboa, Portugal
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**Publicado em:**  
*Proceedings do  
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France (14-16  
September 2004)*

**ABSTRACT** The aim of this work is to show progresses reached with an alternative anodising process for aluminium and aluminium alloys, based in sulphuric/boric baths, under different operating conditions. Traditional processes of chromic acid anodising and sulphuric acid anodising were used as reference. The corrosion resistance of the anodised materials was determined by electrochemical impedance spectroscopy and outdoor exposure. The present results show that a good protection is achieved with the sulphuric/boric process. The structure of the oxide films formed on AA2024 with the different anodising processes and its dependence on the anodising and sealing parameters were investigated by scanning electron microscopy and transmission electron microscopy and compared in order to interpret their corrosion performance. The films formed on commercial aluminium using the same anodising conditions were also investigated, as a way for assessing the influence of the alloying elements.

Photoelectrochemical spectroscopy and capacitance measurements were used to assess the electronic properties of anodic oxide films formed by the different processes, in order to obtain information on the electronic structure of these films. The results obtained indicate that the oxide films formed on aluminium show a semiconductive behaviour, with bandgap energies that are identical for the oxides studied, despite their different characteristics. Moreover, from the capacitance measurements performed on commercial aluminium it is possible to ascribe an n-type semiconductive behaviour, in accordance to the literature. It was found out that capacitance measurements may be used as a valuable technique for the assessment of the quality of anodised layers, allowing the distinction between an efficient and an inefficient sealing. Therefore, they may be used to predict the corrosion resistance of these materials.

# A INDÚSTRIA ENERGÉTICA E OS PROJECTOS DE EQUIPAMENTOS PARA A PRODUÇÃO DE ENERGIA

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**Mestrado em:** Gestão de Projectos

**Grau Concedido por:** Universidade Aberta

**Orientador:** Prof. Vieitas, José Maciel

**Mestrado Concluído em:** 21 de Janeiro de 2004

A globalização dos mercados, tem introduzido transformações várias a nível económico, político e social, em diversos sectores de actividade. As transformações acontecidas, têm-se estendido a múltiplos sectores de actividade, como o sector energético, o qual tem uma importância relevante, pela sua relação estreita com importantes factores, que podem ser constrangedores da evolução económica e social, nomeadamente entre outros, a consciência agora existente da finitude dos combustíveis fósseis, o consumo e economia de energia e as novas preocupações de carácter ambiental.

A transformação acelerada dos mercados, induz à necessidade de mudança organizacionais, realçando-se a crescente importância da identificação de factores críticos, que conduzem ao aumento da competitividade e produtividade, como forma das empresas alcançarem resultados superiores aos da concorrência.

Face às transformações nos mercados, à mudança organizacional e à identificação dos factores críticos de sucesso mencionados, o objectivo deste estudo, é analisar, como é efectuada a gestão de projectos na Divisão das Centrais Térmicas e Controlo Ambiental (DCTCA) do Grupo Asea Brown Boveri (ABB) Portugal, SA, sendo certo, que a gestão dos projectos de equipamentos para a produção de energia e controlo Ambiental, efectuada nesta empresa, é um factor crítico muito importante, pelo seu impacte nos resultados finais dos contratos, na garantia da qualidade e na satisfação dos clientes. Para efectuar esta análise, começou por analisar-se o sector energético em geral e as questões relacionadas, com a economia de energia, no sentido de avaliar a importância e o mercado existente, para as empresas fabricantes de equipamentos para a produção de energia e controlo ambiental.

Para gerir um projecto, é importante conhecer o produto e as suas características. Para tal, fizemos uma abordagem aos aspectos tecnológicos dos equipamentos para a produção de energia ( conhecidos por geradores de vapor ) e controlo ambiental e por fim analisámos a própria ABB/DCTCA, no que se refere à organização, mercados, etc. e a metodologia seguida na gestão dos seus projectos.

Dos resultados alcançados com este estudo, referimos a necessidade de introdução de melhorias, nos processos tecnológicos, para aproveitar as sinergias existentes no Grupo ABB e gerir os projectos de modo mais integrado, para, se necessário, introduzir correcções em tempo real, recorrendo para tal a um melhor apetrechamento de tecnologias de informação.

# METODOLOGIA DE MANUTENÇÃO DE UM AVIÃO COMERCIAL

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**Mestrado em:** Manutenção Industrial

**Grau Concedido por:** Faculdade de Engenharia da Universidade do Porto

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**Mestrado Concluído em:** 13 de Janeiro de 2004

As características específicas do transporte aéreo comercial obrigam a que se dê uma particular importância a um conjunto alargado de variáveis, com especial relevo para a segurança da operação, sendo parte integrante desta, os programas de manutenção e a sua execução. Ao longo dos tempos os conceitos, as metodologias e os procedimentos utilizadas na definição dum programa de manutenção de um avião sofreram alterações, que nunca colocaram em causa os seus objectivos nomeadamente, os de evitar a degradação dos níveis de segurança de operação e de fiabilidade inerente ao material de voo, o de restabelecer os níveis iniciais de segurança e fiabilidade, uma vez constatada a sua degradação e o de cumprir os requisitos referidos, com o mínimo de custo possível.

Este trabalho, visa numa primeira fase, introduzir o tema, identificar as diferentes entidades que emitem e regulamentam a actividade da manutenção, definindo os objectivos e conteúdos dos programas de manutenção, bem como a metodologia seguida para a sua elaboração e certificação.

Na segunda fase do trabalho pretende-se de uma forma prática comparar metodologias de planeamento e execução dum programa de manutenção de um avião, identificando oportunidades de reduções de custos de manutenção bem como da possibilidade de aumento de facturação correspondente a uma maior disponibilidade dos aviões.

Desta forma encontraram-se oportunidades de melhoria, que tornam as empresas mais competitivas, para fazerem face ao mercado, que após a desregulamentação, e com o advento dos operadores designados por low cost carriers, se tornou fortemente competitivo.



04

# ENGENHARIA QUÍMICA

Anuário Científico 2004

ISEL



# THE SYNTHESIS OF NOVEL POLYMER-BOUND CALIX[4]ARENES

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Two simple and efficient procedures for the synthesis of linear and cross-linked polymers containing hydrophobic and hydrophilic lower rim derivatives of *p*-*tert*-butylcalix[4]arenes are described. The target polymers were prepared either through the direct attachment of 25,26,27,28-tetrahydroxy-*p*-*tert*-butylcalix[4]arene (**1**), or its tripropoxy (**2**) and tetracarboxymethoxy (**4**) derivatives, to lightly cross-linked Merrifield's resins (1-2% DVB) or via radical addition copolymerisation of 25,26,27-tripropoxy-28-(4-vinyl-benzyloxy)-*p*-*tert*-butylcalix[4]arene (**11**) with styrene and a cross-linking agent.

**Publicado em:**  
*Reactive & Functional  
Polymers*, 2004, 61,  
147-151.

# MULTIPERIOD SYNTHESIS AND OPERATIONAL PLANNING OF UTILITY SYSTEMS WITH ENVIRONMENTAL CONCERNS

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**Publicado em:**  
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Chemical Engineering,*  
2004, 28, 745-753.

Utility plants supply the required energy demands to industrial processes. Several authors were addressed the synthesis and design of those plants. However, a multiperiod model for utility systems including environmental concerns wasn't described until now.

This paper presents an extension of Iyer and Grossmann (1997, 1998) model to synthesis and multiperiod operational planning in order to include the global emissions of atmospheric pollutants issues coming from the fuels burning.

A new five steps algorithm is introduced to solve this multiobjective model. One motivation example enables us to compare the different units and fuel selection and also the operation periods of an industrial utility system taking in account the electrical power import/export policy and environmental concerns.

# INFLUENCE OF THE CHEMICAL COMPOSITION OF STAINLESS STEELS ON THE ELECTRONIC STRUCTURE OF PASSIVE FILMS FORMED IN ARTIFICIAL SEA WATER

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The electronic structure of passive films formed on stainless steels of different chemical composition in artificial sea water is examined by capacitance measurements (Mott-Schottky approach) and photo-electrochemistry. Analytical characterization is carry out by Auger Electron Spectroscopy. The influence of the main alloying elements (Cr, Ni) on the development of space charge regions, which can be described as a depletion or accumulation layers are discussed.

**Publicado em:**

*Portugaliae*

*Electrochimica Acta*  
(2004) 22, 263-278

# COMPARATIVE ELECTROCHEMICAL BEHAVIOUR OF THE COMPLEXES TRANS[Mo(NCN){NCNC(O)R}(DPPE)<sub>2</sub>]Cl (R = Et OR Ph) AND TRANS [Mo(NCN)Cl(DPPE)<sub>2</sub>][BF<sub>4</sub>]

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The bis(cyanoimide) complex *trans*-[Mo(NCN)<sub>2</sub>(dppe)<sub>2</sub>] (**1**, dppe = Ph<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>) is susceptible of electrophilic attack to form the acylated and aroylated derivatives *trans*-[Mo(NCN){NCNC(O)R}(dppe)<sub>2</sub>]Cl (R = Et **2a** or Ph **2b**). Herein, we report a preliminary study on the electrochemical behaviour of complexes **2** and the derivative *trans*-[Mo(NCN)Cl(dppe)<sub>2</sub>][BF<sub>4</sub>] **3**, as investigated by cyclic voltammetry (CV) and controlled-potential electrolysis (CPE), what has allowed a comparison of the electron-donor ability of the ligands.

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Portugaliae  
*Electrochim. Acta.*,  
2004, 22, 19-23.

# SYNTHESES AND PROPERTIES OF Re(III) COMPLEXES DERIVED FROM HYDROTRIS (1-PYRAZOLYL)METHANES: MOLECULAR STRUCTURE OF $[\text{ReCl}_2(\text{HCpz}_3)(\text{PPh}_3)][\text{BF}_4]$

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The complexes  $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})(\text{PPh}_3)_2]$  **1** (Hpz = pyrazole),  $[\text{ReCl}_2\{\text{N}_2\text{C}(\text{O})\text{Ph}\}(\text{Hpz})_2(\text{PPh}_3)]$  **2**,  $[\text{ReCl}_2(\text{HCpz}_3)(\text{PPh}_3)][\text{BF}_4]$  **3** and  $[\text{ReCl}_2(3,5\text{-Me}_2\text{Hpz})_3(\text{PPh}_3)]\text{Cl}$  **4** were obtained by treatment of the chelate  $[\text{ReCl}_2\{\eta^2\text{-}N,O\text{-N}_2\text{C}(\text{O})\text{Ph}\}(\text{PPh}_3)_2]$  **0** with hydrotris(1-pyrazolyl)methane  $\text{HCpz}_3$  (**1,3**), pyrazole Hpz (**1,2**), hydrotris(3,5-dimethyl-1-pyrazolyl)methane  $\text{HC}(3,5\text{-Me}_2\text{pz})_3$  (**4**) or dimethylpyrazole  $3,5\text{-Me}_2\text{Hpz}$  (**4**). Rupture of a  $\text{C}(sp^3)\text{-N}$  bond in  $\text{HCpz}_3$  or  $\text{HC}(3,5\text{-Me}_2\text{pz})_3$ , promoted by the Re centre, has occurred in the formation of **1** or **4**, respectively. All compounds have been characterized by elemental analyses, IR and NMR spectroscopy, FAB-MS spectrometry, cyclic voltammetry and, for **1**,  $\text{CH}_2\text{Cl}_2$  and **3**, also by single crystal X-ray analysis. The electrochemical  $E_L$  Lever parameter has been estimated, for the first time, for the  $\text{HCpz}_3$  and the benzoyldiazenide  $\text{NNC}(\text{O})\text{Ph}$  ligands.

**Publicado em:**

*J. Organomet. Chem.*,  
2004, in press.

# ASSAY FOR GLUCOSE OXIDASE FROM ASPERGILLUS NIGER AND PENICILLIUM AMAGASAKIENSE BY FOURIER TRANSFORM INFRARED SPECTROSCOPY

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*Analytical Biochemistry*, vol. 333, p. 320-327.

A simple and direct assay method for glucose oxidase (EC 1.1.3.4) from *Aspergillus niger* and *Penicillium amagasakiense* was investigated by Fourier transform infrared spectroscopy. This enzyme catalyzed the oxidation of D-glucose at carbon 1 into D-glucono-1,5-lactone and hydrogen peroxide in phosphate buffer in deuterium oxide ( $D_2O$ ). The intensity of the D-glucono-1,5-lactone band maximum at 1212  $cm^{-1}$  due to C-O stretching vibration was measured as a function of time to study the kinetics of D-glucose oxidation. The extinction coefficient  $\epsilon$  of D-glucono-1,5-lactone was determined to be 1.28  $mM^{-1} cm^{-1}$ . The initial velocity is proportional to the enzyme concentration by using glucose oxidase from both *A. niger* and *P. amagasakiense* either as cell-free extracts or as purified enzyme preparations. The kinetic constants ( $V_{max}$ ,  $K_m$ ,  $k_{cat}$ , and  $k_{cat}/K_m$ ) determined by Lineweaver–Burk plot were  $433.78 \pm 59.87 U mg^{-1} protein$ ,  $10.07 \pm 1.75 mM$ ,  $1095.07 \pm 151.19 s^{-1}$ , and  $108.74 s^{-1} mM^{-1}$ , respectively. These data are in agreement with the results obtained by a spectrophotometric method using a linked assay based on horseradish peroxidase in aqueous media:  $470.36 \pm 42.83 U mg^{-1} protein$ ,  $6.47 \pm 0.85 mM$ ,  $1187.77 \pm 108.16 s^{-1}$ , and  $183.58 s^{-1} mM^{-1}$  for  $V_{max}$ ,  $K_m$ ,  $k_{cat}$ , and  $k_{cat}/K_m$ , respectively. Therefore, this spectroscopic method is highly suited to assay for glucose oxidase activity and its kinetic parameters by using either cell-free extracts or purified enzyme preparations with an additional advantage of performing a real-time measurement of glucose oxidase activity.

# THE USE OF FOURIER TRANSFORM INFRARED SPECTROSCOPY TO ASSAY FOR UREASE FROM PSEUDOMONAS AERUGINOSA AND CANAVALLIA ENSIFORMIS

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A novel assay method was investigated for urease (EC 3.5.1.5) from *Pseudomonas aeruginosa* and *Canavalia ensiformis* by Fourier transform infrared spectroscopy. This enzyme catalyzed the hydrolysis of urea in phosphate buffer in deuterium oxide ( $D_2O$ ). The intensities of the bicarbonate bands maxima at 1625 and 1365  $cm^{-1}$  and of the amide I band at 1605  $cm^{-1}$  were measured as a function of time to study the kinetics of urea hydrolysis. The extinction coefficients of urea and bicarbonate were determined to be 0.72, 0.48, and 0.56  $mM^{-1} cm^{-1}$  at 1625, 1605, and 1365  $cm^{-1}$ , respectively. The initial velocity is proportional to the enzyme concentration by using the ureases from both *C.ensiformis* and *P. aeruginosa*. The kinetic constants ( $V_{max}$ ,  $K_m$ , and  $K_{cat}$ ) determined by Lineweaver–Burk plot were 532.2 U  $mg^{-1}$  protein, 6.4 mM, and 806.36  $s^{-1}$ , respectively. These data are in agreement with the results obtained by a spectrophotometric method using a linked assay based on glutamate dehydrogenase in aqueous media. Therefore, this spectroscopic method is highly suited to assay for urease activity and its kinetic parameters by using either cell-free extracts or purified enzyme preparations with an additional advantage of performing a real-time measurement of urease activity.

**Publicado em:**

*Analytical Biochemistry*, vol. 331, p. 115-121.

# DETOXIFICATION - THE ROLE OF MUSHROOM NUTRITION

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**Publicado em:**  
*Mycology News*, 1 (9),  
p.7- 8.

A number of pathological damages including carcinogenesis and cellular degeneration related to aging are due to reactive oxygen species (ROS), or superoxide radicals. These reactive oxygen species are produced by sunlight, ultraviolet radiation, chemical reactions, as well as by metabolic processes, and are toxic to living cells since they oxidize and degrade important biological macromolecules such as lipids and proteins (1). Health maintenance and the avoidance of chronic degenerative conditions therefore depends to a large extent on the body's ability to neutralise, in other words detoxify, such ROS. Central to the body's battle against ROS are a number of enzyme systems, prominent among which is Superoxide dismutase (SOD), which catalyses the destruction of superoxide radicals and hence protects oxygen-metabolizing cells from the harmful effect of these free radicals. Several research workers have shown that SOD is involved in diseases such as Parkinson's disease, cancer and anemia (1,2). Another important enzyme system is cytochrome "P-450" which is located in the endoplasmic reticulum and plays an important role in metabolism and detoxification of endogenous substances (3). In addition, enzyme therapy has been shown to play an important role in several clinical conditions including cancer, malignant lymphomas and cardiovascular disorders (4,5). Mushrooms have been known to possess medicinal properties for thousands of years and higher basidiomycete mushrooms have been used in clinical nutrition for their anti-tumour, immune modulating, cardiovascular and anti-microbial effects (6). As well as other complex substances of therapeutic interest, such as protein-bound polysaccharide complexes (i.e PSK, PSP and Lentinan) and secondary metabolites (i.e terpenes, alkaloids and lactones) we are now finding that mushrooms are rich sources of many enzymes. Several mushrooms have been shown to contain substances which mimic SOD activity (7) and the "P450" cytochrome enzyme system has also been found in some higher basidiomycete fungi. Other enzymes present in clinically used mushrooms include laccase, glucose oxidase and peroxidase (8). It is likely that the potent enzymatic and ROS detoxifying properties of mushrooms are in large

part due to the harsh environments colonized by mushroom mycelia with high concentrations of free radicals that the mushrooms have to protect themselves against. In this connection it is worth noting that these enzymes are found almost exclusively in the mushroom mycelia and hence preparations derived from the fruiting bodies of mushrooms are likely to have far lower levels of enzymatic activity than those derived from mushroom mycelia. In the present work, we investigated the levels of SOD, cytochrome "P450", cytochrome "P450" reductase (NADPH dependent) and secondary thrombin inhibiting metabolites in the following mushrooms: *Coriolus versicolor*, *Cordyceps sinensis*, *Ganoderma lucidium (Reishi)* and *Grifola frondosa (Maitake)*. There are a number of secondary metabolites in mushrooms which play an important role as thrombin inhibitors (10) and since thrombin is an important protease of the coagulation system it is a suitable target for inhibition of blood coagulation, which is desirable in combating many age related conditions.

# SUPPRESSION OF A CHARGE-DENSITY-WAVE GROUND STATE IN HIGH MAGNETIC FIELDS: SPIN AND ORBITAL MECHANISMS

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125113 (2004)

The charge density wave (CDW) transition temperature in the quasi-one-dimensional (Q1D) organic material  $(\text{Per})_2\text{Au}(\text{mnt})_2$  is relatively low ( $T_{\text{CDW}} \sim 12$  K). Hence in a mean field BCS model, the CDW state should be completely suppressed in magnetic fields of order 30–40 T. To explore this possibility, the magnetoresistance of  $(\text{Per})_2\text{Au}(\text{mnt})_2$  was investigated in magnetic fields to 45 T for  $0.5 \text{ K} < T < 12 \text{ K}$ . For fields directed along the Q1D molecular stacking direction,  $T_{\text{CDW}}$  decreases with field, terminating at about  $\sim 37$  T for temperatures approaching zero. Results for this field orientation are in general agreement with theoretical predictions, including the field dependence of the magnetoresistance and the energy gap,  $\Delta_{\text{CDW}}$ . However, for fields tilted away from the stacking direction, orbital effects arise above 15 T that may be related to the return of un-nested Fermi surface sections that develop as the CDW state is suppressed. These findings are consistent with expectations that Q1D metallic behavior will return outside the CDW phase boundary. ©2004 *The American Physical Society*

# HIGH MAGNETIC FIELD INDUCED CHARGE DENSITY WAVE STATE IN A QUASI-ONE-DIMENSIONAL ORGANIC CONDUCTOR

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The quasi-one-dimensional organic conductor  $(\text{Per})_2\text{Pt}(\text{mnt})_2$  exhibits a charge density wave ground state below 8 K. Magnetoresistance and magnetization measurements show that the charge density wave is suppressed with magnetic fields of order 20 T, above which a high resistance state, with a cascade of subphases, appears. This new state, tentatively identified as a field induced charge density wave, reenters a low resistance state above 40 T. The results are presented in light of theoretical work [D. Zanchi *et al.* Phys. Rev. B 53, 1240 (1996).] involving field induced charge density wave ground states in high magnetic fields. ©2004 *The American Physical Society*

**Publicado em:**

*Phys. Rev. Lett.* 93,  
076406 (2004)

# ANALYTICAL CHARACTERISATION AND CORROSION BEHAVIOUR OF BIS-[TRIETHOXSILYLPROPYL]TETRASULPHIDE PRE-TREATED AA2024-T3

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This work aims at studying the corrosion behaviour of AA2024-T3 pre-treated with bis-[triethoxysilylpropyl]tetrasulphide. Simultaneously, the work investigates the influence of the Cu-rich intermetallic particles on the formation of the silane film. The analytical characterisation of the silane films was performed by Auger electron spectroscopy and X-ray photoelectron spectroscopy. The corrosion performance of the pre-treated substrates was evaluated by electrochemical impedance spectroscopy. Atomic force microscopy associated with Kelvin probe was also used to determine the influence of the silane film on the Volta potential distribution on the alloy surface. The results show that copper present in the intermetallics plays an important role on the film formation.

**Publicado em:**

*Corrosion Science*,  
2005, 47, 869-881  
(Available online 22  
September 2004)

# SOLVATION EFFECTS IN THE HETEROLYSES OF 3-X-3-METHYLPENTANES (X=CL, BR, I)

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A comparative study of the heterolysis reactions of 3-X-3-methylpentanes (X=Cl, Br, I) in a set of protic and aprotic solvents was performed at 25.00 °C. Rate constant values were correlated with solvent descriptors using the TAKA multiparametric equation. Our results point towards a decrease in both hydrogen bond donor acidity (electrophilicity) and hydrogen bond acceptor basicity (nucleophilicity) contributions, and towards an increase in the dipolarity/polarizability term on going from the chloride substrate to iodide. These features suggest the formation of an increasingly early transition state, in contrast to the classical Hughes–Ingold rationale, but in agreement with the Hammond postulate. Furthermore, there seems to be no evidence for a shift in solvation from an electrophilic (or anionic) mode in the chloride substrate to a nucleophilic (or cationic) mode in the iodide, as claimed by some authors.

**Publicado em:**

*Journal of Physical  
Organic Chemistry,*  
2004, 17, 1061-1066.

# TRANSFORMATION OF N-HEXANE ON PtAl/MCM-41 AND PtAl/SBA-15

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PtAl/MCM-41 and PtAl/SBA-15 materials were prepared by post-synthesis alumination followed by introduction of platinum by ion exchange. The samples were characterized by pyridine adsorption followed by FTIR and TPR of hydrogen. The catalytic behavior was explored in the transformation of n-hexane.

**Publicado em:**

*React. Kinet. Catal. Lett.* , 2004, 82, 139-147.

# SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF PIGMENTS FROM ANNATTO SEEDS (EXPERIMENTS AND MODELING).

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Annatto (*Bixa orellana*) is a tropical tree whose seeds produce pigments, with hues from yellow to red. Among other applications, these colors are used in the food industry to improve cheese, margarine and butter. One of the main pigments existing in the pericarp of the seeds is the carotenoid bixin ( $C_{25}H_{30}O_4$ ), which is one of the main natural colors, and it is found only in this plant. Chemically is the mono-methyl ester of the dicarboxylic acid norbixin, another important pigment found in annatto seeds.

Supercritical  $CO_2$  extraction of the pigments from annatto seeds was carried out at pressures of 200 bar and at temperature of 40 °C, in a flow apparatus, at two flow rates of fluid (0.67g/min and 1.12g/min). The efficiency of the extraction was low (about 1 % of the pigments were extracted). The increase in flow rate led to a decrease in extraction efficiency. A great increase in the yield (from 1% to 45%) was achieved using supercritical carbon dioxide, containing 5mol% of ethanol, as extraction fluid at pressures of 200 and 300 bar and temperatures of 40 and 60 °C. Although the temperature and the pressure led to an increase in yield, the changes in the flow rate seemed do not influence it. Furthermore, two plug flow models were applied to describe the supercritical extraction of the pigments from annatto seeds. In these models is considered that the axial dispersion is negligible and that the properties of the solvent and seeds bed remain unaltered. It was observed that the presence of ethanol in the supercritical phase modified the mass transfer regime, possibly due to modifications in vegetable behavior. In this case, experimental data were well represented by a model in which the mass transfer is controlled by the solvent film. On the other hand, the experimental data with pure carbon dioxide were well represented by a model in which the intra-particle mass transfer controls the process. Mass transfers coefficients were determined and compared well with those obtained by other workers with similar models for the supercritical extraction of solutes from plant materials.

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# OPTIMIZAÇÃO DO TRATAMENTO TERCIÁRIO DE ÁGUAS RESIDUAIS EM LAGOAS DE ESTABILIZAÇÃO POR UTILIZAÇÃO DE UM GRANULADO DE ARGILA EXPÂNDIDA COMO SUPORTE PARA FIXAÇÃO DE BIOMASSA BACTERIO-ALGAL: ESTUDO LABORATORIAL

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As lagoas de estabilização são, por definição, um processo de tratamento natural que decorre em reactores biológicos que, em termos físicos e de princípios de funcionamento, em tudo se assemelham aos ecossistemas naturais. As lagoas terciárias são normalmente concebidas para tratar o efluente secundário de processos de tratamento convencionais ou de lagunagem, com objectivos de desinfecção e de remoção de nutrientes. O estado da arte do tratamento terciário de águas residuais em lagoas de estabilização indica como principais limitações à sua aplicação mais efectiva, a presença de elevadas concentrações de biomassa microalgal suspensa no efluente final e a inconsistência de desempenho no que respeita à remoção de nutrientes. Por outro lado, a instalação de suportes para fixação de biomassa perifítica nas lagoas vem sendo defendida como uma via que poderá permitir não só ultrapassar em grande parte aquelas limitações, como também incrementar significativamente a remoção de azoto total neste sistemas. Trata-se de uma tecnologia recente e ainda em desenvolvimento, relativamente à qual a literatura refere fundamentalmente estudos realizados à escala laboratorial ou piloto e utilizando materiais artificiais como suporte.

O presente estudo teve como objectivo investigar as potencialidades de utilização de um material natural, um granulado de argila expandida (GrAE), como suporte para fixação de biomassa bacterio-algal em lagoas terciárias e avaliar o seu efeito na eficiência do tratamento.

Os resultados obtidos, em ensaios realizados à escala laboratorial, permitiram concluir boa viabilidade do GrAE para fixação do biofilme bacterio-algal, bem como uma melhoria global do tratamento terciário, decorrente da sua instalação no reactor. Verificou-se não só um incremento significativo na remoção de azoto total (+ 25%) e de CQO, como também uma marcada redução nas concentrações de biomassa microalgal suspensa no efluente final. A maior remoção de azoto total é atribuída a uma intensificação do mecanismo de nitrificação/desnitrificação no reactor, relacionável com a presença do biofilme no GrAE e traduzida pelas reduzidas concentrações de azoto amoniacal e nitratos registadas no efluente final.

# OPTIMIZAÇÃO DA REMOÇÃO DE AZOTO EM LAGOAS TERCIÁRIAS POR UTILIZAÇÃO DE UM SUPORTE GRANULAR DE ARGILA EXPANDIDA PARA FIXAÇÃO DE BIOMASSA BACTERIO-ALGAL

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O estado da arte do tratamento terciário de águas residuais em lagoas de estabilização indica como principais limitações à sua aplicação mais efectiva, a presença de elevadas concentrações de biomassa microalgal suspensa no efluente final e a inconsistência de desempenho no que respeita à remoção de nutrientes. Por outro lado, a instalação de suportes para fixação de biofilme bacterio-algal nas lagoas (lagoas de biomassa fixa) vem sendo defendida como uma via que poderá permitir não só ultrapassar significativamente aquelas limitações, como também incrementar significativamente a remoção de azoto total nestes sistemas. Trata-se de uma tecnologia recente e ainda em desenvolvimento, relativamente à qual a literatura refere fundamentalmente estudos realizados à escala laboratorial ou piloto e utilizando materiais artificiais como suportes.

O presente estudo teve como objectivo investigar as potencialidades de utilização de um material natural, um granulado de argila expandida (GrAE), como suporte para fixação de biomassa bacterio-algal em lagoas terciárias e avaliar o seu efeito na eficiência do tratamento.

O estudo foi realizado à escala laboratorial em dois reactores com diferentes condições de regime hidráulico, funcionando em paralelo e continuamente alimentados por uma água residual sintética (CQO:N:P=40:31:8) simulando as condições de um efluente secundário. Foram realizados dois ensaios, antes e após a instalação do suporte em estudo (GrAE) nos reactores, durante os quais se procedeu à caracterização dos seguintes parâmetros de controlo em amostras do volume total de 24 horas dos efluentes (10-11 amostras/reactor em cada ensaio), de acordo com os métodos recomendados no *Standard Methods* (APHA,1989): pH, CQO, N-total, N-Kjeldhal, N-NH<sub>4</sub><sup>+</sup>, N-NO<sub>3</sub><sup>-</sup>, N-NO<sub>2</sub><sup>-</sup>, P-total, P-PO<sub>4</sub><sup>3-</sup>, SST e clorofila *a*. Os resultados obtidos permitiram concluir boa viabilidade do GrAE para fixação do biofilme bacterio-algal, o qual se desenvolveu de acordo com um padrão de comportamento semelhante ao habitualmente descrito para suportes artificiais neste tipo de sistemas, bem como uma melhoria global do tratamento terciário, decorrente da sua instalação no reactor. Verificou-se não só um incremento significativo

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na remoção de azoto total e de CQO, como também uma marcada redução nas concentrações de biomassa microalgal suspensa no efluente final. A maior remoção de azoto é fundamentalmente atribuída a uma intensificação do mecanismo de nitrificação/desnitrificação, relacionável com a presença do biofilme no GrAE e traduzida pelas reduzidas concentrações de azoto amoniacal e nitratos registadas no efluente final, particularmente para um dos regimes hidráulicos estudados.

# MONITORIZAÇÃO DE CICLOS DE NITRIFICAÇÃO/DESNITRIFICAÇÃO

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A consciencialização da sociedade de que é necessário proteger os recursos hídricos disponíveis tem aumentado nas últimas décadas. A actividade agro-pecuária é uma das mais poluentes, nomeadamente as suiniculturas, na medida em que as suas águas residuais contêm concentrações significativas de matéria orgânica e de nutrientes. A presença excessiva de nutrientes nos recursos hídricos constitui um enorme problema, face aos seus efeitos nocivos, pelo que, nos últimos anos têm sido impostos limites legais cada vez mais restritivos, quer em termos de matéria orgânica quer em termos de nutrientes.

Os sistemas de tratamento de efluentes com concentrações elevadas de azoto, mais divulgados, baseiam-se em processos biológicos que incorporam a nitrificação e a desnitrificação. A remoção biológica de azoto é condicionada por diversos parâmetros, pH, temperatura, C/N e presença de substâncias inibidoras.

Neste estudo procurou-se averiguar a influência de diversos parâmetros na fase de nitrificação e de desnitrificação no sistema de tratamento de efluente de suinicultura, através de monitorização de CQO,  $N_{\text{amoniaco}}$ ,  $\text{NO}_x$ , pH,  $\text{O}_2$  e da relação C/N. No presente trabalho, foram utilizados reactores de biomassa suspensa, do tipo SBR (Sequencing Batch Reactor) com arejamento intermitente, obtendo-se assim alternadamente condições aeróbias e anóxicas.

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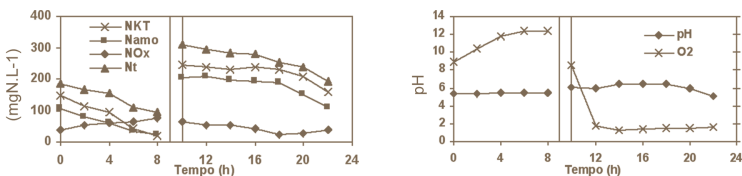


Figura 1. Evolução de parâmetros num ciclo de desnitrificação/nitrificação – Ensaio 3

# NITRIFICAÇÃO PARCIAL DO AZOTO AMONIAICAL

**Santos, M<sup>a</sup> Teresa<sup>1</sup>; Trindade, Teodoro P.<sup>1</sup>;  
Manuel, Renato E.<sup>2</sup>; Amaral, Leonor M.<sup>2</sup>**

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8<sup>a</sup> Conferência  
Nacional de Ambiente,  
Lisboa, Portugal,  
Outubro de 2004.*

Nas últimas décadas tem-se verificado uma crescente preocupação com as questões ambientais, em parte resultantes das pressões sociais existentes. Dada a necessidade de proteger os recursos hídricos têm sido impostos limites legais cada vez mais exigentes.

Apesar do desenvolvimento, nos últimos anos, dos sistemas de tratamento de águas residuais, em Portugal ainda existe pouca capacidade instalada para remover a quantidade de nutrientes necessária ao cumprimento da legislação em vigor. A remoção de azoto pode ser realizada por processos físico-químicos ou biológicos, no entanto os primeiros apresentam geralmente desvantagens relativamente aos segundos.

Os processos biológicos de remoção de azoto consistem essencialmente em nitrificação e desnitrificação, apresentando-se, geralmente como a via mais económica de controlar o azoto existente em águas residuais.

Nos últimos anos surgiram dois novos processos biológicos denominados “SHARON” (Single Reactor for High Ammonium Removal Over Nitrite) e “ANAMMOX” (Anaerobic Ammonium Oxidation) destinados à remoção de azoto em águas residuais fortemente carregadas. Tendo em conta a variedade de factores envolvidos e a diversidade de águas residuais, existe um enorme espaço de investigação/experimentação, por forma a garantir o correcto ajuste das condições operatórias a situações específicas.

O presente estudo tem como principal objectivo: a análise de sensibilidade do sistema aos principais parâmetros operatórios e avaliação da sua capacidade de nitrificação parcial do azoto amoniacal.

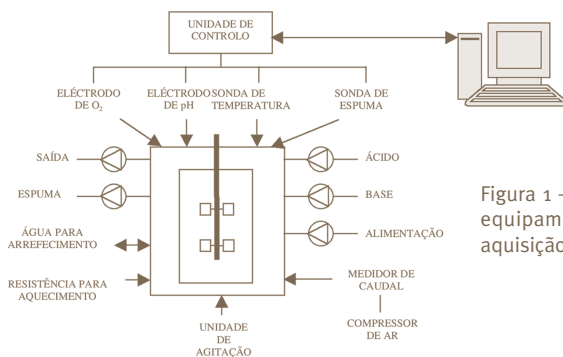


Figura 1 – Reactor e respectivos equipamentos de controlo e aquisição de dados

# DETERMINAÇÃO DE INCERTEZAS EM MÉTODOS DE ANÁLISE NÃO ROTINEIROS USANDO “BUILDING BLOCKS”

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Importantes decisões são tomadas com base nos resultados de análises analíticas e é importante avaliar a qualidade desses resultados. A validação de um resultado como suporte à decisão é impossível sem o conhecimento da incerteza associada ao resultado. De extraordinária importância, a incerteza associada a um resultado analítico não é evidente nem fácil de calcular. Por definição a incerteza de uma medida consiste num “parâmetro associado ao resultado de uma medida, que caracteriza a dispersão de valores associados ao valor medido”. Por exemplo o erro associado à determinação de uma concentração  $c$  que depende de  $x_1, \dots, x_n$  variáveis é dado por:

$$\Delta[c(x_1, \dots, x_n)] = \sum_{i=1}^n \left( \frac{\partial c}{\partial x_i} \right) \Delta x_i \quad (1)$$

Para  $x_1, \dots, x_n$  independentes, a incerteza  $u_c$  associada à concentração será dada por:

$$u_c^2[c(x_1, \dots, x_n)] = \sum_{i=1}^n \left( \frac{\partial c}{\partial x_i} \right)^2 u_{x_i}^2 \quad (2)$$

Face à complexidade das situações reais, várias aproximações têm sido propostas para o cálculo das incertezas associadas às determinações analíticas: a aproximação ISO (conhecida como a aproximação “bottom-up”), o método proposto pelo *Analytical Methods Committee* (aproximação “top-down”) e a estimativa da incerteza baseada na informação obtida a partir de processos de validação.

Neste trabalho utiliza-se a aproximação “bottom-up” para calcular as incertezas associadas a processos de digestão, por microondas e por via clássica. Analisaram-se amostras ambientais (folhas de choupo e solos) a partir das quais se determinam teores de metais pesados através de GFAAS.

Foi usada uma folha de cálculo com um elevado detalhe na especificação de cada componente de incerteza. Pode assim ser usada como “building blocks” para cálculos posteriores de incerteza em que essa componente está presente. Consegue-se deste modo agilizar o cálculo da incerteza em métodos de análise não rotineiros onde o cálculo da incerteza associada aos resultados é geralmente evitada face à complexidade dos cálculos.

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# LINEAR AND CROSSLINKED COPOLYMERS OF P-TERT-BUTYLCALIX[4]ARENE DERIVATIVES AND STYRENE: AN APPROACH TO POLYMER-BOUND CALIX[4]ARENES

Barata, Patrícia D.; Costa, Alexandra I.; Mendes, Ana R.; Gregório, Carla C.; Prata, José V.

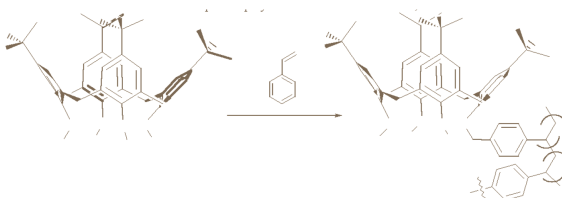
Secção de Química Orgânica, Departamento de Engenharia Química, Instituto Superior de Engenharia de Lisboa, Lisboa, Portugal.

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Livro Electrónico de Resumos e <http://poco4.icpf.cas.cz> / do 11th International Conference on Polymers and Organic Chemistry, Praga, República Checa, Julho 2004.

Calixarenes are a class of synthetic receptor molecules that possess intramolecular bow-shaped cavities capable of accommodate guest molecules and ions. In recent years, the interesting properties shown by these cyclic oligomeric compounds have stimulated the exploitation of useful methods towards their incorporation into polymeric matrices, given its interest for the development of selective electrodes and membranes, chemical and biochemical sensors and selective extraction processes.

In this communication we will report on the synthesis and characterisation of new polymeric materials obtained through the radical addition copolymerisation of *p*-*tert*-butylcalix[4]arene derivatives, possessing one or more vinylic units, with styrene and divinylbenzene. In particular, when calixarene **1** ( $R_1=R_2=R_3=Pr$ ) and styrene in various feed ratios were reacted, soluble copolymers **3a** were obtained. Their composition (calculated from the  $^1H$ NMR) showed good correlation with the feeding ratios used (1:10 and 1:20; calixarene:styrene) and analogous conversions were achieved within 24h of reaction. Insoluble polymeric matrices (**3b**) were also prepared through the same technique, using divinylbenzene as crosslinker. The weight-average molar mass of the linear copolymers ranging from 19000 to 41000  $gmol^{-1}$ , as determined by GPC, and showed low polydispersity. As expected, higher glass transition temperatures were obtained for the crosslinked polymers (DSC analysis). The tethering of two polymerisable vinyl units to *p*-*tert*-butylcalix[4]arene (**2**) followed by copolymerisation with styrene, leading ultimately to calixarene-based crosslinked copolymers, will also be discussed.



# CALIXARENOS SUPOSTADOS EM POLÍMEROS – SÍNTESE DE CALIX[4,6,8]ARENOS LIGADOS A POLIESTIRENO ENTRECruzADO

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Os calixarenos são macromoléculas cíclicas que possuem uma cavidade intramolecular capaz de desenvolver interacções selectivas com iões ou espécies moleculares. Como consequência desta característica, a síntese de calixarenos covalentemente ligados a suportes poliméricos tem sido alvo de desenvolvimentos recentes. Tendo em vista a sua aplicabilidade na extracção em fase sólida de espécies moleculares e biomoleculares e como catalisadores de transferência de fase, foi desenvolvida muito recentemente uma nova metodologia sintética para a preparação de diversos polímeros contendo *p*-*tert*-butilcalix[4]arenos com derivados hidrofílicos e hidrofóbicos na coroa inferior. Tal metodologia permitiu, de modo simples e eficaz, a obtenção de polímeros funcionais, cuja capacidade de reconhecimento de espécies moleculares presentes em soluções aquosas foi entretanto determinada. De modo a avaliar a extensão e aplicabilidade do método a calixarenos contendo 6 e 8 unidades fenólicas por macrociclo, alargando desse modo o conjunto de potenciais aplicações dos polímeros obtidos, foi realizado o presente estudo. Os polímeros **5-7** foram obtidos por ligação directa a resina Merrifield (PS-DVB 1% clorometilado) na presença de base, com grau de incorporação entre 50 a 65%. O teor de incorporação mássica da unidade de calixareno foi avaliado para diferentes razões molares de resina e calixareno. Estes materiais foram posterior-mente transformados nos ésteres e ácidos correspon-dentes. A incorporação directa na resina do derivado **4** foi igualmente realizada, permitindo desse modo avaliar o grau de entrecruzamento ocorrido durante a ligação dos calixarenos **1-3** à resina, usando as mesmas condições reaccionais.

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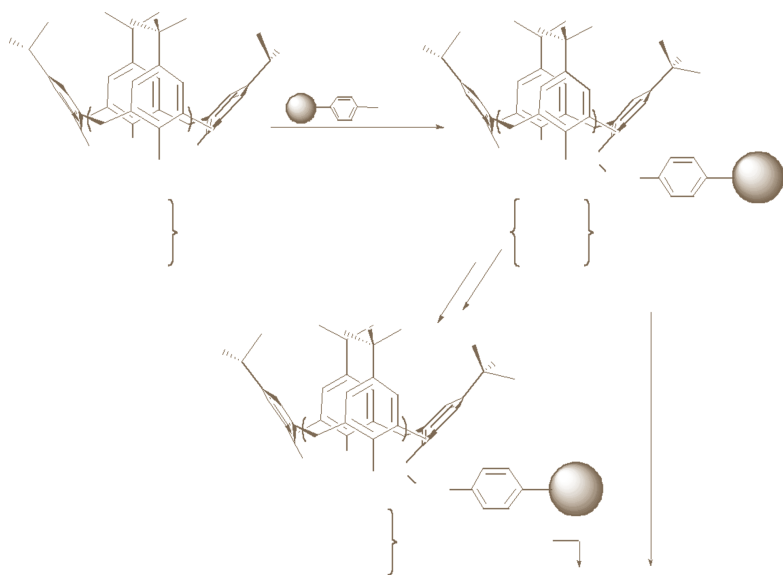


Fig. 1- Incorporação de unidades de *p*-*tert*-butilcalix[4-8]arenos em matrizes poliméricas insolúveis.

# SÍNTESE E CARACTERIZAÇÃO DE COPOLÍMEROS LINEARES E ENTRECruzADOS DE DERIVADOS DE *p*-TERT-BUTILCALIX[4]ARENO E ESTIRENO

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Os calixarenos constituem uma importante classe de oligómeros cíclicos sintéticos cuja capacidade de reconhecimento de espécies moleculares e iónicas, está associada à sua conformação e ao tamanho da cavidade do macrociclo. A associação de calixarenos a suportes poliméricos, conjugando as capacidades específicas de reconhecimento dos primeiros com a robustez mecânica e inércia química das resinas, levou ao desenvolvimento destes polímeros. Estudos recentes conduziram à preparação de novos materiais poliméricos contendo unidades de *p*-tert-butilcalix[4]arenos por vias sintéticas distintas.

Na comunicação que se apresenta será descrita a síntese e caracterização de copolímeros lineares e entrecruzados obtidos por polimerização em suspensão de uma unidade de calixareno adequadamente funcionalizada (**1**) com estireno.

O monómero **1** foi sujeito a polimerização radicalar em condições diversas (tempo de reacção, relação monómero **1**:estireno e quantidade de iniciador) conduzindo à obtenção de polímeros lineares ( $T_g = 120\text{-}140^\circ\text{C}$ ;  $M_w = 19000\text{-}41000 \text{ gmol}^{-1}$ ). Realizando a copolimerização na presença de um agente de *crosslinking*, usando a técnica de polimerização por suspensão, foram obtidos polímeros entrecruzados (**2c**) ( $T_g = 141^\circ\text{C}$ ). Estes resultados serão confrontados com os obtidos para o polímero resultante da ligação directa de *O*-tripropil-*p*-tert-butilcalix[4]areno a resina Merrifield (poliestireno-DVB 1% clorometilado) ( $T_g = 149^\circ\text{C}$ ).

A metodologia utilizada possibilita o controlo de diversos parâmetros cruciais para as propriedades do polímero final obtido, destacando-se o grau de incorporação, a massa molecular, o grau de entrecruzamento e a porosidade.

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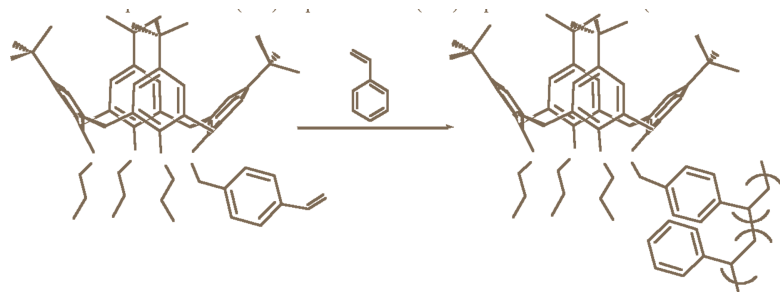


Fig. 1- Copolimerização do derivado vinílico de *O*-tripropil-*p*-*tert*-butilcalix[4]areno com estireno.

# MECHANISM STUDIES ON THE AZIRIDINATION REACTION OF OLEFINS CATALYZED BY PALLADIUM(II) USING BROMAMINE T AS THE NITROGEN SOURCE

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Aziridines form an attractive class of compounds available by a variety of procedures. We have previously reported our preliminary results of a novel PdCl<sub>2</sub>-assisted aziridination of olefins both simple and electron-deficient, with bromamine T (TsNBrNa), easily prepared, cheap and stable as the nitrogen transfer reagent. To clarify the mechanism of this reaction, several deuterio olefins were prepared (Scheme 1) through different methodologies and submitted to the reaction conditions.



Based on experimental results obtained with deuterated olefins, a mechanism involving the formation of a Pd<sup>+4</sup> palladocycle after the *syn* addition to the olefin of a bromamine T-Pd species is proposed. The results suggest that the reaction is strongly dependent on the ability of olefin substitute coordination with a postulated Pd(IV) intermediate.

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*Livro de Resumos do V Congresso International de Química e Ingeniería Química, Havana, Cuba, Novembro 2004.*

# THE USE OF BTESPT FILMS AS CHROMATE SUBSTITUTE FOR PRE-TREATMENTS ON AA2024-T<sub>3</sub>.

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 EUROCORR 2004 -  
 Long Term Prediction  
 & Modelling of  
 Corrosion – EFC event  
 nº 266, Nice, France,  
 Setembro 2004*

This work investigates a surface pre-treatment for the Aluminium alloy 2024-T<sub>3</sub> based on the use organosilanes. The treatment consists in the immersion of the substrate into a water/alcohol solution of bis-[triethoxysilypropyl]tetrasulfide (BTESPT). This pre-treatment aims at replacing the conventional chromating process on AA2024-T<sub>3</sub>.

Electrochemical Impedance Spectroscopy (EIS) and salt spray testing (SST) were used to evaluate the anticorrosive ability of this treatment on the AA2024-T<sub>3</sub>. Analytical characterization of the silane films was performed by Auger Electron Spectroscopy (AES) and X-Ray photoelectron Spectroscopy (XPS). In addition, ellipsometry was used to assess film thickness. SEM analyses were also carried out in order to study the film microstructure.

The results demonstrated that the corrosion protection performance of the silane pre-treatment is comparable to that of chromate and that the copper present in the intermetallics plays an important role on the film formation.

# SÍNTESE, CARACTERIZAÇÃO E ESTRUTURA DE RAIOS X DOS ISÓMEROS TRANS E CIS- [RuCl(p-NCC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>)(PMe<sub>3</sub>)<sub>4</sub>]PF<sub>6</sub>

Gandum, C.<sup>1</sup>; Vertlib, V.<sup>1</sup>; Rodrigues, J.<sup>1</sup>; Garcia, M.H.<sup>2,3</sup>; Robalo, M.P.<sup>2,4</sup>; Nattinen, K.<sup>5</sup>; Rissanen, K.<sup>5</sup>

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Os materiais opticamente não lineares (ONL) constituem uma área de crescente interesse científico e tecnológico, em resultado das suas potenciais aplicações na indústria optoelectrónica e fotónica. Os complexos de metais de transição com ligandos orgânicos com sistemas conjugados oferecem várias e interessantes possibilidades de combinação dos efeitos ONL, com as propriedades electrónicas (e.g. redox e magnéticas), para a preparação de novos materiais multifuncionais. Na continuação de trabalhos anteriores nesta área, apresentam-se os mais recentes resultados da síntese e caracterização de complexos deste tipo, no caso do [RuCl(p-NCC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>)(PMe<sub>3</sub>)<sub>4</sub>]PF<sub>6</sub> e dos seus respectivos isómeros *trans* e *cis*. Os estudos de UV-Vis. e RMN confirmam a maior estabilidade em solução do isómero *cis*, cuja conversão em diclorometano é acelerada pela acção da luz. Os complexos foram caracterizados por FTIR, RMN de <sup>1</sup>H, <sup>13</sup>C e <sup>31</sup>P, UV-Vis., MS e por difracção de raios X.

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*Livro de Resumos do XIX Encontro da Sociedade Portuguesa de Química, Coimbra, Portugal, Abril de 2004.*

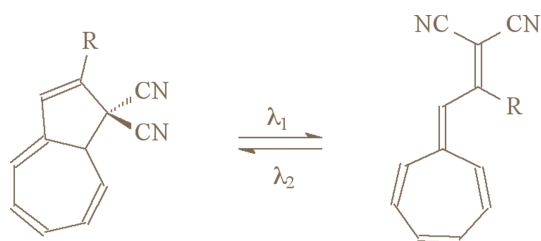
# SYNTHESIS OF NEW IRON(II) DIHYDROAZULENE MOLECULAR MATERIALS IN VIEW TO PHOTOCHROMIC PROPERTIES

Coelho, C.<sup>1</sup>; Ribeiro, P.<sup>2</sup>; Pacheco, V.<sup>2</sup>; Pontinha, A.<sup>2</sup>; Robalo, M.P.<sup>1,2</sup>; Garcia, M.H.<sup>1,3</sup>; Dias, A.R.<sup>1</sup>

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Photochromic molecules have attracted much attention from fundamental and practical points of view due to their potential for applications to optical devices such as optical memories and switches. Although several organic photochromic molecules has been studied, photochromic systems involving transition metal complexes has been very little explored. Nevertheless, the role of the transition metal centres has found to be relevant in the intramolecular photosensitization of the photochromic process.

In the present communication we report the synthesis and functionalisation of dihydroazulene type molecules, known as light molecular switches, since irradiation can be used for the conversion of non-conjugated (or "OFF") to conjugated (or "ON") forms. The coordination of these chromophores to iron(II) fragments,  $[\text{Fe}(\eta^5\text{-C}_5\text{H}_5)(\text{dppe})]$  and  $[\text{Fe}(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2]$  lead to a new family of compounds. The new complexes were characterised by the usual spectroscopic IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR techniques. Studies by UV/Vis spectroscopy were performed in order to characterise the photochromic behaviour of the new complexes.



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 Conference on  
 Organometallic  
 Chemistry (ICOMC),  
 Vancouver, Canadá,  
 Julho de 2004.*

# MOLECULAR STRUCTURE AND CRYSTAL PACKING OF CpMR ISONITRILES (M = Ru, Fe; R = PHOSPHINES AND TMEDA). HOW TO OBTAIN NEW SOLIDS FOR NLO

Piedade, M.F.M. da<sup>1,2</sup>; Dias, A.R.<sup>1</sup>; Duarte, M.T.<sup>1</sup>;  
Florindo, P.<sup>2</sup>; Garcia, M.H.<sup>1,2</sup>; Rodrigues, J.C.<sup>3</sup>;  
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Organometallic compounds have found great importance in the area of non linear optical materials, due to their significant values of second and third harmonic generation. This has been possible owing to the diversity of metal centres, oxidation states, ligands and geometries. We present here a systematic study on Fe and Ru isonitrile derivatives, where we try to emphasize the relationship between molecular design and crystal engineering: the metal centers have been enriched and depleted by changing the type and number of ligands, the  $\pi$  systems have been extended and different counter ions have been used. The effects that this diversity has promoted in the 3D crystal packing will be discussed and compared.

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22nd European  
Crystallography  
Meeting, Budapeste,  
Hungria, Agosto de  
2004.*

# DENSITY FUNCTIONAL THEORY CALCULATIONS ON $\eta^5$ -MONOCYCLOPENTADIENYLME-TAL COMPLEXES WITH CONJUGATED NITRILE CHROMOPHORES

Ramalho, J.P. Prates<sup>1</sup>; Candeias, A. Estevão<sup>2</sup>  
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Congresso  
Internacional de  
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Porto, Portugal,  
Setembro de 2004.*

During the past decade, the interest on organometallic compounds for the development of novel nonlinear optical (NLO) materials with large second-order nonlinearities has considerably increased in view of their potential application in the area of integrated optics. Experimental and computational investigations utilizing quantum theory afforded useful insights concerning the molecular structural requirements necessary to induce large second-order nonlinearity response. The strategy to obtain these properties has been the synthesis of compounds with highly polarizable asymmetric structures through the existence of delocalized electronic system bridge (chromophore) between an electron-withdrawing and electron-donating group. Recent experimental work on  $\eta^5$ -monocyclopentadienylmetal complexes with *p*-substituted benzonitrile and oligothiophene nitrile chromophores showed a correlation between the first hyperpolarizability (*b*) and the communicability between the chromophores and the organometallic fragments. In addition, some EHMO calculations on nickel and iron complexes have corroborate that the larger values of experimental hyperpolarizability correspond to lower HOMO-LUMO gaps. In order to get a better understanding on the electronic factors that may be responsible for the second-order nonlinear optical behavior of  $[\text{CoCp}(\text{dppe})(\text{p-NCC}_6\text{H}_4\text{R})]^{2+}$  and  $[\text{FeCp}(\text{dppe})(\text{NC}\{\text{SC}_4\text{H}_2\}_n\text{NO}_2)]^+$  complexes and their correlation with experimental spectroscopic and electrochemical data, density functional theory calculations were made in the model complexes  $[\text{CoCp}(\text{H}_2\text{PCH}_2\text{CH}_2\text{PH}_2)(\text{p-NCC}_6\text{H}_4\text{R})]^{2+}$  and  $[\text{FeCp}(\text{H}_2\text{PCH}_2\text{CH}_2\text{PH}_2)(\text{NC}\{\text{SC}_4\text{H}_2\}_n\text{NO}_2)]^+$  (*n*=1,2). Especial emphasis was given to the HOMO-LUMO gaps and their character. Spatial localization of electron charge by means of topological analysis of the electron localization function (ELF) has been performed to gain insight into the nature of the chromophores binding to the metal centers.

# REACTIONS OF CYANAMIDE AND DERIVED CYANOIMIDE AT A MOLYBDENUM DIPHOSPHINIC CENTRE

Martins, L.M.D.R.S.<sup>1,2</sup>; Silva, T.F.S.<sup>2</sup>;  
Cunha, S.M.P.R.M.<sup>1</sup>; Alegria, E.C.B.A.<sup>1,2</sup>;  
Silva, M.F.C. Guedes da<sup>1,3</sup>; Pombeiro, A.J.L.<sup>1</sup>

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Cyanamide,  $N\equiv CNH_2$ , is a small organonitrogen molecule with industrial, biological and environment interest. There has also been a recent growth of interest in complexes containing the cyanoimide (NCN) ligand, due to their potential applications in catalysis, as precursors for metal nitrides or carbonitrides, or intermediates for organocyanamides.

In pursuit of our interest in the coordination and activation of cyanamide by transition metal centres, we have investigated the reactions of the cyanamide-derived bis(cyanoimide) complex of Mo(IV) *trans*-[Mo(NCN)<sub>2</sub>(dppe)<sub>2</sub>] (**1**, dppe = Ph<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>Ph<sub>2</sub>) with various electrophiles.

In **1**, the N<sub>β</sub> of only one of the two cyanoimide ligands is susceptible of attack by acid chlorides, RC(O)Cl (R = alkyl or aryl), or trialkyloxonium salts, [R<sub>3</sub>O][BF<sub>4</sub>] (R = alkyl), affording the corresponding addition products *trans*-[Mo(NCN){NCNC(O)R}(dppe)<sub>2</sub>]Cl (**2**, R = alkyl or aryl) or *trans*-[Mo(NCN)(NCNR)(dppe)<sub>2</sub>][BF<sub>4</sub>] (**3**, R = alkyl).

Protonation of complexes **3** affords the products with the ligated alkylcyanamide *trans*-[Mo(NCN)(NCNHR)][BF<sub>4</sub>]<sub>2</sub> (**4**, R = Et or Me), whereas complexes **2**, on reaction with various electrophiles, lead to the formation of the new mono(cyanoimide) species *trans*-[Mo(NCN)Cl(dppe)<sub>2</sub>][BF<sub>4</sub>] (**5**) with liberation of the corresponding acylcyanamides.

A stopped-flow spectrophotometric study of latter reactions is being performed and the kinetic data are discussed.

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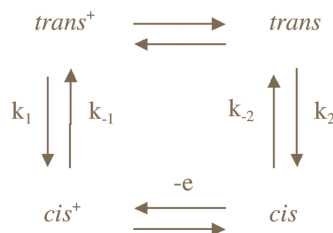
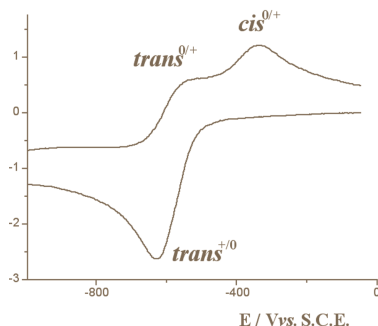
# ISOMERIZAÇÃO GEOMÉTRICA INDUZIDA POR TRANSFERÊNCIA ELECTRÓNICA DE COMPLEXOS *trans* DE MOLIBDÊNIO E CIANOIMIDA

Alegria, E.C.B.A.<sup>1,2</sup>; Cunha, S.M.P.R.M.<sup>1</sup>;  
Martins, L.M.D.RS.<sup>1,2</sup>; Silva, M.F.C. Guedes da<sup>1,3</sup>;  
Pombeiro, A.J.L.<sup>1</sup>

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Efectuou-se o estudo do comportamento electroquímico dos complexos *trans*-[Mo(NCN){NCNC(O)R}(dppe)<sub>2</sub>]Cl (R = Me ou Et) (representados por *trans*<sup>+</sup>) por voltametria cíclica (VC) e electrólise a potencial controlado (EPC) em meio aprótico, utilizando um eléctrodo de Pt. Estes complexos exibem, para além de uma onda anódica parcialmente reversível atribuível à oxidação de Mo(IV) a Mo(V), um primeiro processo de redução parcialmente reversível (*trans*<sup>+</sup> a *trans*<sup>0</sup>) que envolve uma isomerização *trans*-*cis* induzida por transferência electrónica (Figura) de acordo com o esquema indicado de tipo ECEC em quadrado. A simulação digital dos dados de voltametria cíclica numa determinada gama de velocidades de varrimento permite fazer uma estimativa das correspondentes constantes de equilíbrio e de velocidade.

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Americana de  
Electroquímica,  
Universidad de Costa  
Rica, Fevereiro de  
2004



# ALKYLATION OF CYANOIMIDO AT A N<sub>2</sub>-BINDING MOLYBDENUM CENTRE

Martins, L.M.D.R.S.<sup>1,2</sup>; Alegria, E.C.B.<sup>1,2</sup>;  
Cunha, S.M.P.R.M.<sup>1</sup>; Silva, M.F.C. Guedes da<sup>1,3</sup>;  
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In pursuit of our studies on the activation of small molecules with biological interest by transition metal centres, in particular on the coordination chemistry of the cyanamide (N≡C-NH<sub>2</sub>) at the molybdenum N<sub>2</sub>-binding site *trans*-[Mo(dppe)<sub>2</sub>] (dppe = Ph<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>), we obtained the bis(cyanoimido) complex *trans*-[Mo(NCN)<sub>2</sub>(dppe)<sub>2</sub>].<sup>1</sup> Prompted by the observation that the latter complex undergoes ethylation at one of the cyanoimido ligands by the oxonium Et<sub>3</sub>O<sup>+</sup>, we decided to investigate its reactivity towards alkyl halides. The alkylated complexes *trans*-[Mo(NCN)(NCNR)(dppe)<sub>2</sub>]X (X = I or Br, R = linear or branched alkyl) were obtained and characterized by IR and multinuclear NMR spectroscopies, FAB<sup>+</sup>-MS spectrometry, elemental analysis, and electrochemical methods.

The electrophilic addition occurs on the *exo*-N atom, confirmed by the X-ray crystal structure of *trans*-[Mo(NCN)(NCNMe)(dppe)<sub>2</sub>], as shown in Figure 1, which shows a linear multiple-bond coordination of the NCN and NCNMe ligands.

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de 2004*

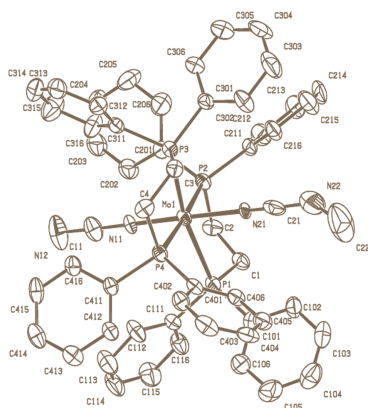


Figure 1 - X-ray crystal structure of *trans*-[Mo(NCN)(NCNMe)(dppe)<sub>2</sub>].

# CLEAVAGE OF A C(sp<sup>3</sup>)-N BOND IN HYDROTRIS(PYRAZOLYL)METHANE PROMOTED BY A Re-BENZOYLHYDRAZIDO COMPLEX. CRYSTAL STRUCTURE OF [ReCl<sub>2</sub>{NNC(O)C<sub>6</sub>H<sub>5</sub>} (NNC<sub>3</sub>H<sub>4</sub>)(PPh<sub>3</sub>)<sub>2</sub>]

Alegria, E.C.B.<sup>1,2</sup>; Martins, L.M.D.R.S.<sup>1,2</sup>; Silva, M.F.C. Guedes da<sup>1,3</sup>; Pombeiro, A.J.L.<sup>1</sup>

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There is a current growth of interest in complexes containing the tripodal ligands tris(pyrazolyl)borates and the neutral isoelectronic tris(pyrazolyl)alkanes due to their importance in synthetic inorganic, bioinorganic and organometallic chemistries.

In pursuit of our interest in the interaction of pyrazole-containing molecules with various metal ions, we have been studying the reactions of [HBpz<sub>3</sub>]<sup>+</sup> (pz = pyrazolyl) and [HB(3,5-Me<sub>2</sub>pz)<sub>3</sub>]<sup>+</sup> with Fe(II)<sup>1</sup>, Cu(I) and Cu(II) sites, and now we report the extension of the study to the reaction of the less investigate hydrotris(pyrazolyl)methane with the benzoylhydrazido-Re(V) chelate species [ReCl<sub>2</sub>{=NN=C(Ph)O-}(PPh<sub>3</sub>)<sub>2</sub>]. The later undergoes the chelate ring opening with coordination of a pyrazole ligand derived from the rupture of a C(sp<sup>3</sup>)-N bond in hidrotris(pyrazolyl)methane, leading to the benzoyldiazenido-Re(III) [ReCl<sub>2</sub>{NNC(O)C<sub>6</sub>H<sub>5</sub>}(NNC<sub>3</sub>H<sub>4</sub>)(PPh<sub>3</sub>)<sub>2</sub>]. Its synthesis and characterization by IR and multinuclear NMR spectroscopies, X-ray diffraction, FAB<sup>+</sup>-MS spectrometry, elemental analysis and electrochemical methods is reported. For comparison, the reaction of [ReCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>{=NN=C(Ph)O-}] with pyrazole itself has been investigated under various conditions.

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*Livro de Abstracts do III EuChem Conference on Nitrogen Ligands in Organometallic Chemistry and Homogeneous Catalysis, Camerino, Itália, Setembro de 2004*

# THEORETICAL INVESTIGATIONS OF THE ELECTROCHEMICAL BEHAVIOUR OF THE COMPLEX TRANS-[FeH(CNH)(dppe)<sub>2</sub>]<sup>+</sup>

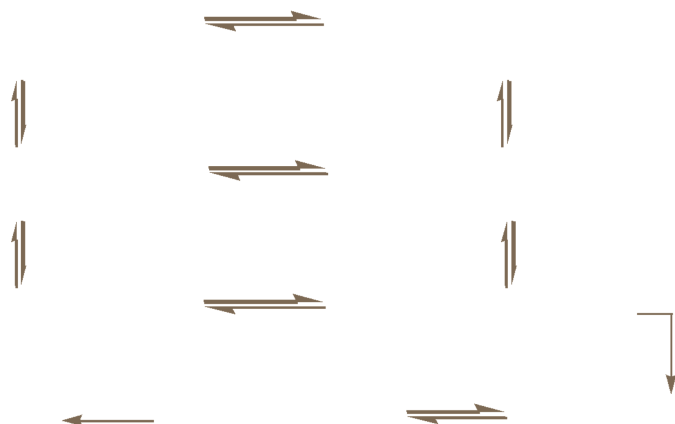
Almeida, Sílvia S.P.R.<sup>1,3</sup>; Kuznetsov, Maxim L.<sup>2,3</sup>  
Pombeiro, Armando J.L.<sup>3</sup>

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The electrochemical behaviour of the model hydride iron complex *trans*-[FeH(CNH)(PH<sub>3</sub>)<sub>4</sub>]<sup>+</sup> (**1**<sup>+</sup>) has been investigated by theoretical methods (DFT approximation, ECP on the metal atom). One electron oxidation of **1**<sup>+</sup> results in the formation of the oxidized species **1**<sup>++</sup>. Both **1**<sup>+</sup> and especially **1**<sup>++</sup> convert to the hydride-cyanide complexes *trans*-[FeH(CN)(PH<sub>3</sub>)<sub>4</sub>]<sup>0/+</sup> (**2/2**<sup>+</sup>) instead of the isocyanide ones *trans*-[Fe(CNH)(PH<sub>3</sub>)<sub>4</sub>]<sup>0/+</sup> (**3/3**<sup>+</sup>). The stronger acidic character of the isocyanide than the hydride was interpreted in terms of electrostatic and frontier MO arguments as well as by the lower stability of **3/3**<sup>+</sup> in comparison with **2/2**<sup>+</sup>. Complex **2**<sup>+</sup> undergoes further metal deprotonation with isomerisation to give *cis*-[Fe(CN)(PH<sub>3</sub>)<sub>4</sub>] (**4**). The calculations indicate that upon oxidation, **4** undergoes nucleophilic attack by BF<sub>4</sub><sup>-</sup> to give a fluoro-complex **5**.

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Expressão Latina,  
Porto, Portugal,  
Setembro de 2004*



# MICROWAVE-ASSISTED [2+3] CYCLOADDITION OF NITRONES TO PLATINUM ORGANONITRILES. A PROMISING CLASS OF NEW BIOLOGICAL ACTIVE OXADIAZOLINES AND KETOIMINES

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*III EuChem Conference*  
*on Nitrogen Ligands in*  
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*Chemistry and*  
*Homogeneous*  
*Catalysis”, Camerino,*  
*Itália, Setembro de*  
*2004.*

The 1,3-dipolar cycloaddition reaction between nitrones and unsaturated systems is a powerful method for the organic synthesis of a wide variety of new heterocyclic derivatives structurally related to lactams, indolizidine alkaloids.<sup>1</sup> The new fused bicyclic oxadiazoline species, obtained by Pt(II) and (IV)-mediated and microwave-assisted [2+3] cycloaddition opens up a facile route for the preparation of  $\Delta^4$ -1,2,4-oxadiazoline and their complexes. This method opens up new perspectives for the metal-mediated synthesis of biologically significant heterocyclic species.<sup>2</sup> In the current work we have studied the influence of the nature of the R group of the organonitrile and performed further reactions of the bicyclic oxadiazoline complexes towards the opening of new routes for compounds with synthetic natural significance. Hence, we increased the electron-acceptor character of the R group in the organonitrile ligand at *trans*-[PtCl<sub>2</sub>(RCN)<sub>2</sub>] (R = CH<sub>2</sub>CO<sub>2</sub>Me or CH<sub>2</sub>Cl) instead of an alkyl one, and obtained a weakening effect on the N-O bond towards a ready ring-opening of the bicyclic oxadiazoline complexes, without the need of any catalyst. By this way an unprecedented single-pot synthesis of various ketoimino complexes is achieved. The same products are also obtained upon hydrogenolysis of oxadiazoline complexes. Moreover platinum complexes with *N*-heterocyclic ligands show very promising anticancer activity and this study further provides novel and potential anti-tumor candidates to be tested.

# SYNTHESIS OF HYDROXAMIC ACID IN TTAB REVERSED MICELLES USING AMIDASE FROM PSEUDOMONAS SP.

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2 Instituto Superior de Engenharia de Lisboa, Lisboa, Portugal

Hydroxamic acids derivatives have a wide spectrum of application due to their ion metal chelating capacity, mainly their capacity to inhibit metalloproteinases that are involved in human diseases. These compounds are used in several pharmaceutical drugs. Amidases (E.C. 3.5.1.4) are enzymes that in nature catalyse the hydrolysis of amide bonds in small aliphatic amides but these enzymes also have the capacity to catalyse the acyl group transferase to amines what enlarged the possibility of synthesising several hydroxamic acids derivatives if the acyl acceptor is hydroxylamine. Amidases with this capacity have been isolated mainly from *Pseudomonas* and *Rhodococcus* strains. As the amidase catalysed reaction involves a ping-pong bi-bi mechanism [Fournand, 1998] with the formation of acyl-enzyme complex that can transfer the acyl unit either to an amine or to the water present in the system, it is the kind of reaction to be performed in organic medium in order to diminish the presence of water. Reverse micelles formed in organic medium have been used to encapsulate enzymes in order to catalyse the synthesis of amide bonds with the formation of dipeptides. In these systems the enzyme remains soluble, what avoids problems with mass transfer that could slow down the reaction velocity and they can easily be transformed into a continuous reaction system. In this work the amidase from a *Pseudomonas aeruginosa* gene expressed in *E. coli*, was purified and encapsulated in reverse micelles of the cationic surfactant tetradecyltrimethyl ammonium bromide dissolved in heptane/octanol. The effect of several parameters of the system that could influence the enzymatic activity were analysed. It is the results of this study that are to be presented.

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CERC3 Young  
Chemists' Workshops  
"Biocatalysis", 023,  
p.31, Erlangen,  
Germany, 24-28 de  
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## DIFFERENTIAL CHROMATOGRAPHIC BEHAVIOUR OF MONOCLONAL ANTIBODIES AGAINST WILD-TYPE AND ALTERED AMIDASES ON IMMOBILIZED METAL CHELATES

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Monoclonal antibodies (Mabs) raised against wild-type and altered amidases from *Pseudomonas aeruginosa* were used to study their behaviour on immobilized metal chelates. The adsorption of Mabs of IgG and IgM classes was investigated by using M (II) – IDA metal chelates containing Cu (II), Ni(II), Zn (II), Co (II) and Ca(II) as a function of pH. The adsorption of Mabs to immobilized metal chelates was pH dependent since high adsorption was observed at pH 8.0. The adsorption of Mabs on metal(II)-IDA chelates was due to the available histidine residues on Mabs molecules since the addition of imidazole in the buffer system abolished the binding of Mabs to these columns.

Both classes of Mabs were purified in one step by immobilized metal affinity chromatography (IMAC) on Zn(II)-IDA agarose columns at pH 8.0 with a high recovery of Mab activity as well as purity. Purified preparations of Mabs were apparently homogeneous on native PAGE and SDS-PAGE. The different chromatographic behaviour of Mabs on metal(II)-IDA chelates is apparently due to the number and spatial distribution of available histidine residues on these Mabs molecules.

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# MAGNETIC FIELD DEPENDENT CHARGE DENSITY WAVE PHASES IN A QUASI-ONE DIMENSIONAL ORGANIC CONDUCTOR

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The quasi-one-dimensional organic conductor  $(\text{Per})_2\text{Pt}(\text{mnt})_2$  exhibits a charge density wave (CDW) ground state below 8 K. Magnetoresistance and magnetization measurements show that the CDW is suppressed with magnetic fields of order 20 T, above which a second high resistance state appears. For fields above 45 T, this second state re-enters a low resistance state. This phenomena will be discussed in light of the recent theoretical treatments of the CDW ground state in high magnetic fields, and new results where pressure has been used to increase the interchain coupling will presented.

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# CHARGE DENSITY WAVE TO MIXED DENSITY WAVE PHASE TRANSITION AT HIGH FIELDS

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The ground states of the quasi-one-dimensional (Q1D) organic metal  $(\text{Per})_2\text{M}(\text{mnt})_2$  (where  $\text{M} = \text{Au}$  and  $\text{Pt}$ ) were investigated by transport and magnetization measurements in magnetic fields of 33 and 45 tesla. The low field charge density wave (CDW) transition temperature is suppressed by applied fields and a high field insulating state is introduced. Under the influence of hydrostatic pressure, the high field behavior differs between the  $\text{M} = \text{Au}$  and  $\text{Pt}$  compounds. The results presented will be discussed within the context a contemporary model of high field density wave behavior.

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# BISMUTH-FILM ELECTRODES IN THE SIMULTANEOUS DETERMINATION OF TOXIC METALS IN ENVIRONMENTAL SAMPLES BY SWASV: AN ALTERNATIVE FOR MERCURY-FILM ELECTRODES

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Determination and detection assays of toxic metals, such as Pb(II), Cd(II) and Cu(II), are an area of continuous research interest due to their toxicity to the environment. One of the most used techniques in the determination of these pollutants is Square Wave Anodic Stripping Voltammetry (SWASV). Among the parameters that determine the low detection limits that can be achieved by SWASV, the type of the working electrode is one of the most significant.

Although mercury is a very attractive choice for electrode material because it has a high cathodic potential window, renewable surface and reproducibility behaviour, disadvantages such as its high toxicity must be taken in consideration. Following a general trend of banishing mercury from analytical assays, environmental friendly analytical methods and electrode material are being investigated. Among a wide range of alternative materials, bismuth film electrodes seem to have a stripping performance that compares favorably with mercury electrodes. Also the low toxicity for bismuth is a major advantage.

The present work reports a comparison between the results obtained for the determination of Pb(II), Cd(II) and Cu(II), at ppb levels by SWASV on a Bismuth-film electrode (BiFE) with those obtained for a mercury-film electrode (MFE).

The voltammetric parameters were investigated in order to enhance the sensitivity and repeatability of the measurements. The real samples investigated were tree leaves and soil samples collected in Lisbon, environmental samples with a complex matrix. These experiments confirm that the stripping performance of bismuth films compare to that of mercury electrodes. The applicability and suitability of the BiFE in the determination of toxic metal in real samples, despite the presence of varying levels of matrix interferences, are also demonstrated.

A major advantage of the BiFE, given its stripping behaviour and the fact that bismuth is a more “environmental-friendly” element, is the possibility to develop mercury-free disposable electrodes in field (environmental, clinical or industrial) testing of toxic metals.

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# DETERMINATION OF ESSENTIAL ELEMENTS IN PORTUGUESE LAVANDULA HONEY USING ATOMIC ABSORPTION SPECTROMETRY

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Chemical and physical analysis of foods plays an important role in obtaining the required information for nutritional labelling purposes and also in ensuring its quality attributes. According to the safety requirements, this analysis may involve not only the detection of components which are potentially harmful to health, but also the quantification of other food constituents. For instance, the mineral elements fulfil important biological functions and at the same time contribute to the food flavour and texture. However, in the same food the mineral content can fluctuate greatly depending on climatic factors, agriculture procedures and composition of soil, among others such as the food processing.

In this context, it is worthwhile to provide the quantification of the essential minerals in honeys. Honey is a typical natural product, used worldwide as a basic foodstuff, having a mineral content of about 0,17% and a physical chemical interesting matrix.

In the present work, which is part of an extensive study carried out on honey's composition, three essential minerals, sodium, potassium and calcium, were determined in the *Lavandula* honey by atomic absorption spectrometry.

At first, a lot of honey samples were collected and its physicochemical characterization was performed. The samples were then submitted to a mineralization stage, in order to destroy the organic matter, and its analysis were carried out using a UNICAM-SOLAAR M5 spectrometer with an air/acetylene flame. To avoid the ionisation interferences on the sodium and potassium determination, caesium was added to the samples and calibration solutions. Moreover, adding lanthanum, the phosphate interference on calcium analysis was also eliminated.

The experimental results were in a good agreement with other literature data and allowed a comparison between the sodium, potassium and calcium contents in *Lavandula* honey.

# SYSTEMATIC SOIL SAMPLING PROCEDURE AS A TOOL FOR MODELING URBAN POLLUTION ON THE SOIL/TREE SYSTEM.

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In the last decades and due to human activity, soil pollution levels have suffered a continuous increase. Since almost all kinds of atmospheric pollution have a direct impact in the soils, this system is a major indicator of the global pollution of a site. A detailed knowledge of pollution levels in the soils is of great importance, namely for the correct characterization of the studied locals, relationship with local bioindicators for local pollution modeling and also for the application of remediation strategies. For the correct determination of pollutant levels, in our case, pollution by metals, the sampling procedure is regarded as the first and most important step towards a more comparable and reproducible analysis. Apart the existing ISO guidelines (ISO/DIS 10381-1, 1995) offering optimal instructions for the realization of studies concerning the soil contamination, these guidelines set out only general principles to be observed. As has been evidenced in the Dornach study [1], in the countries of European Union different strategies and guidelines for the soils sampling are used.

In this study, developed since 1999 in the city of Lisbon, we have worked on a systematic approach for sampling soils in order to carry out the study and the modeling of urban pollution by metals. The proposed model is a simple, but very effective tool to keep under control related aspects of the atmospheric pollution, namely: wind and rain direction, proximity of high traffic streets and topology of the local in terms of buildings height. Because one of the major objectives of this study is to establish a relationship between the soil pollution and the pollution detected using tree leaves as bioindicator, the sampling area is centered in a tree trunk. In every sampling area were collected 12 samples (0-20 cm), distributed by 3 circles with 1, 3 and 5 meters radius centered in the tree trunk, following the direction of the four cardinal points. The metal content of each sampling point has been determined by EDXRF and we have made a total of 84 samples and the determination of 23 metals in each sample.

The results showed a systematic behavior towards the sampling strategy and that its interpretation is much clearer than using a random sampling.

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# DETERMINAÇÃO DE INCERTEZAS EM MÉTODOS DE ANÁLISE NÃO ROTINEIROS USANDO “BUILDING BLOCKS”

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Importantes decisões são tomadas com base nos resultados de análises analíticas e é importante avaliar a qualidade desses resultados. A validação de um resultado como suporte à decisão é impossível sem o conhecimento da incerteza associada ao resultado. De extraordinária importância, a incerteza associada a um resultado analítico não é evidente nem fácil de calcular. Por definição a incerteza de uma medida consiste num “parâmetro associado ao resultado de uma medida, que caracteriza a dispersão de valores associados ao valor medido”. Por exemplo o erro associado à determinação de uma concentração  $c$  que depende de  $x_1, \dots, x_n$  variáveis é dado por:

$$\Delta[c(x_1, \dots, x_n)] = \sum_{i=1}^n \left( \frac{\delta c}{\delta x_i} \right) \Delta x_i$$

Para  $x_1, \dots, x_n$  independentes, a incerteza  $u_c$  associada à concentração será dada por:

$$u_c^2[c(x_1, \dots, x_n)] = \sum_{i=1}^n \left( \frac{\delta c}{\delta x_i} \right)^2 u_{x_i}^2$$

Face à complexidade da situações reais, várias aproximações têm sido propostas para o cálculo das incertezas associadas às determinações analíticas: a aproximação ISO (conhecida como a aproximação “bottom-up”), o método proposto pelo *Analytical Methods Committee* (aproximação “top-down”) e a estimativa da incerteza baseada na informação obtida a partir de processos de validação.

Neste trabalho utiliza-se a aproximação “bottom-up” para calcular as incertezas associadas a processos de digestão, por microondas e por via clássica. Analisaram-se amostras ambientais (folhas de choupo e solos) a partir das quais se determinam teores de metais pesados através de GFAAS.

# ANÁLISE DO POTÁSSIO EM MEL MONOFLORAL

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O mel é um produto natural considerado benéfico para a saúde e daí a sua frequente inclusão na dieta alimentar. Em virtude das suas propriedades, é vulgarmente consumido de uma forma natural e usado como adoçante em diversos produtos alimentares.

A composição química do mel é variável, dependendo de muitos factores, tais como o clima e a flora da região onde foi produzido. No entanto, é comum as amostras de mel apresentarem cerca de 81% de carboidratos, 18% de água e 1% de outros compostos, nomeadamente, elementos metálicos, proteínas, aminoácidos, vitaminas e ácidos orgânicos. Em relação à composição mineral do mel, estudos já realizados revelaram um teor médio em elementos metálicos de cerca de 0,17%, do qual fazem parte elementos essenciais como o cálcio, o sódio e o potássio, mas eventualmente também outros como o crómio ou o chumbo, que sendo tóxicos necessitam de ser quantificados e controlados. Nesse sentido, e tendo em conta que existem poucos estudos detalhados sobre a composição mineral de muitos produtos alimentares, foi implementado no Laboratório de Controlo Analítico do ISEL, um programa experimental cujo objectivo é o doseamento de elementos metálicos em alimentos através de espectrometria de absorção atómica. Inicialmente, procedeu-se à caracterização físico-química de sete variedades de mel monofloral produzido em diferentes regiões do País. Os ensaios realizados envolveram a determinação da acidez, índice de refração, conductividade eléctrica e rotação específica, bem como do teor em cinzas e em água, tornando possível um estudo comparativo destas propriedades nos diferentes tipos de mel.

Em seguida e na continuidade dos estudos de quantificação de minerais essenciais no mel, efectuou-se o doseamento do potássio nas diversas amostras, usando um espectrofotómetro de absorção atómica UNICAM-SOLLAR M5 com uma chama de ar/acetileno. O método de análise foi optimizado em termos de intensidade da fonte emissora, caudal de acetileno e altura de queimador. As amostras de mel foram previamente reduzidas a cinzas e solubilizadas numa solução de cloreto de céσιο. Na análise das amostras foi usado o método da curva de calibração, cuja aplicação envolveu também a

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adição de cloreto de cézio a cada uma das soluções padrão utilizadas. De uma forma geral, os resultados das análises efectuadas mostraram uma boa concordância com valores indicados por outros autores e possibilitaram efectuar uma comparação quanto ao teor em potássio presente nos diferentes tipos de mel monofloral produzido em Portugal.

# VOLTAMETRIA DE REDISSOLUÇÃO ANÓDICA EM AMOSTRAS AMBIENTAIS DE MATRIZ COMPLEXA. O PROBLEMA DA LIMPEZA DO FILME DE MERCÚRIO.

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A voltametria de Redissolução Anódica (ASV) tem como uma das suas principais aplicações a análise de catiões metálicos em soluções de matriz complexa. O método consiste essencialmente num passo de pré-concentração da espécie electroactiva na superfície de um eléctrodo de trabalho, a um valor de potencial fixo. Segue-se um passo de determinação da espécie onde se aplica um varrimento de potencial anódico de modo a provocar a reoxidação dos metais acumulados no eléctrodo. Obtém-se como resultado uma relação directamente proporcional entre a corrente medida e a concentração da espécie em análise. Entre cada ciclo de concentração/determinação, procede-se à limpeza electroquímica do filme de mercúrio, por aplicação de um valor de potencial fixo e durante um determinado tempo, de modo a garantir a remoção completa de algum vestígio de metal que não tenha sido reoxidado durante o varrimento de potencial. Esta possibilidade acentua-se à medida que a concentração em espécie electroactiva aumenta, sendo necessário tempos de limpeza sucessivamente superiores. No entanto o excessivo tempo de limpeza pode levar a uma degradação do filme de mercúrio havendo várias propostas para a sua protecção. Caso não se efectue este procedimento, a leitura dos valores de corrente nos ciclos seguintes será afectada de um erro. O problema torna-se ainda mais relevante quando se analisam amostras reais (folhas de árvore e amostras de solo) devido aos efeitos de matriz. A complexidade desta dificulta os processo de acumulação e reoxidação da espécie electroactiva bem como da formação da amálgama entre o mercúrio e o metal depositado. O tempo de limpeza do filme revela-se assim uma variável de significativa importância e que deverá ser cuidadosamente optimizado.

Neste trabalho apresentam-se os resultados de um estudo de optimização do tempo de limpeza do filme de mercúrio face a diferentes concentrações de Pb (II). Pretende-se assegurar a reprodutibilidade das condições de ensaio para cada ciclo de determinação garantindo assim uma análise rigorosa.

O filme mercúrio foi depositado na superfície de um disco de carbono vítreo utilizando-se uma concentração de  $5 \times 10^{-5}$  mol.L<sup>-1</sup> em Hg (II).

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Testou-se a gama de concentrações de Pb(II) entre  $5 \times 10^{-8}$  mol.L<sup>-1</sup> e  $5 \times 10^{-7}$  mol.L<sup>-1</sup>.

Os resultados obtidos mostram que um inadequado tempo de limpeza do filme de mercúrio produz erros significativos nos teores de metal determinados por ASV. O procedimento de optimização e validação do tempo de limpeza deverá ser considerado como um parâmetro merecedor de investimento experimental para a garantia da reprodutibilidade e qualidade dos resultados.

# INFLUÊNCIA DE ACTIVIDADE ANTRÓPICAS NA COMPOSIÇÃO DE SOLOS NA REGIÃO DE LISBOA.

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Nas últimas décadas tem-se vindo a verificar uma acumulação de resíduos no ambiente, como resultado do aumento da população e das actividades industriais. Um dos grupos de contaminantes do meio ambiente são os metais, que não são facilmente removidos do ambiente. Este trabalho tem como objectivo o estudo químico de amostras de solos recolhidas em zonas urbanas, da cidade de Lisboa, com características distintas e sujeitas a diferentes tipos de poluição, nomeadamente em Monsanto, em Belém e em Cabo Ruivo (I.S.E.L.). Os locais de amostragem foram seleccionados tendo em conta:

- 1.** Belém - zona de lazer muito utilizada sujeita a uma elevada intensidade de tráfego da marginal Lisboa-Cascais;
- 2.** Cabo Ruivo - uma elevada densidade populacional numa zona residencial;
- 3.** Monsanto - uma zona de lazer protegida no meio do parque.

Em cada um destes locais foram recolhidas 12 amostras de superfície (0-20 cm) a partir do centro de um círculo definido por uma árvore, segundo uma recta a 1, 3 e 5m do centro, na direcção dos 4 pontos cardeais e a para posterior análise.

Foi efectuada uma caracterização multielementar por espectrometria de fluorescência de raios-X dispersiva de energias, que é um método de análise química instrumental que permitiu a determinação simultânea e não destrutiva, de um elevado número de elementos químicos constituintes dos solos, como o Mg, Al, Si, S, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Br, Rb, Sr, Y, Zr, Nb, Pb.

Os resultados obtidos mostram diferenças significativas nos locais estudados. Assim, nas zonas sujeitas a um maior tráfego automóvel (Belém e Cabo Ruivo) detectaram-se os níveis mais elevados de Pb e ainda de contaminação em Cu e Zn. No caso de Monsanto, aparentemente, não foi detectada contaminação. No entanto, a composição química revelou a existência de um solo mais produtivo, de “natureza” basáltica (teores elevados de V, Cr, Fe), que é regularmente utilizado na construção e manutenção de jardins.

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# CÁLCULO DE INCERTEZAS: FOLHA DE CÁLCULO VERSUS PROGRAMA DEDICADO

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A realização de análises quantitativas em laboratórios químicos conduz à obtenção de resultados analíticos cuja credibilidade necessita de ser validada, já que importantes decisões são tomadas com base nestes resultados. A validação de um resultado, como suporte à decisão, é impossível sem o conhecimento da incerteza associada ao próprio resultado. Para avaliar a incerteza é necessário identificar as várias fontes de incerteza e quantificá-las. Dependendo da quantidade de fontes de incerteza a incluir, o esforço de cálculo envolvido pode ser considerável, tornando o processo difícil e moroso se realizado manualmente. Este esforço é ainda mais notório nos métodos de análise não rotineiro como são os processos de investigação.

De modo a fazer face à complexidade das situações procurou-se facilitar o cálculo das incertezas desenvolvendo no nosso laboratório duas aplicações informáticas: uma folha de cálculo (EXCEL) e um programa dedicado (Visual Basic), ambos para o cálculo de incertezas.

Na folha de cálculo em EXCEL foi usado um elevado detalhe na especificação de cada componente de incerteza. Pode assim ser usada como “building blocks” para cálculos posteriores de incerteza em que essa componente está presente.

Na aplicação em Visual Basic encontram-se incluídos os componentes de incerteza já referidos que permite a total liberdade na sua definição para um qualquer processo de análise não rotineiro. Do programa faz também parte um módulo para a determinação de incertezas em processos de análise rotineiros concebido sob a forma de assistente.

Da análise das soluções propostas conclui-se que na utilização da folha de cálculo o utilizador tem todo o controlo sobre o conteúdo, interface, equações e algoritmo, e pode facilmente pôr em causa a segurança e integridade dos dados. No entanto esta é uma ferramenta de utilização comum de aceitação imediata como instrumento de cálculo. O programa apresenta-se como uma solução bastante sólida para a resolução do problema de cálculo de incertezas. Constitui-se, no entanto, como uma solução fechada não sendo possível a alteração total dos seus modelos de cálculo pré-definidos.

As duas soluções propostas poderão coexistir devido ao facto que

para análise não rotineira o recurso à folha de cálculo é bastante mais interessante devido a poderem ser utilizados blocos de cálculo. Para processos rotineiros, o recurso a um programa “fechado” parece-nos uma solução mais adequada.

# DESEMPENHO DE METAIS DISPERSOS EM ZEÓLITOS COMO ELÉCTRODOS NA REACÇÃO DE ELECTRÓLISE DA ÁGUA. COMPARAÇÃO COM MATERIAIS CLÁSSICOS.

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A electrólise é o processo no qual a energia eléctrica é usada para forçar a ocorrência de uma reacção química não espontânea. Na electrólise da água esta decompõe-se em hidrogénio e oxigénio. Este processo apresenta-se como a forma mais eficaz de produção de gases de elevada pureza, sendo de principal importância a produção de hidrogénio nestas condições uma vez que este pode ser convertido em electricidade utilizando células de combustível. Uma vez que a decomposição da água nos seus constituintes não é um processo espontâneo é necessário formar uma pilha na qual uma solução aquosa ácida ou básica constitui o electrólito, sendo os eléctrodos utilizados normalmente de material inerte como a grafite ou de um metal pouco reactivo como a platina. No caso da platina o processo é mais eficiente, apesar deste material ser muito mais dispendioso. Assim, este trabalho teve por objectivo a procura de novos eléctrodos que pudessem aliar a maior eficácia do processo ao menor custo. Foram utilizados como eléctrodos materiais microporosos – zeólitos –, nos quais foram dispersas micropartículas de platina, funcionando estas como a componente electroactiva. Os zeólitos são silicoaluminatos cristalinos com estrutura microporosa cujas propriedades têm vindo a ser exploradas nos domínios da catálise e da adsorção. No entanto, apesar destes materiais se apresentarem como isolantes, funcionam como suporte para espécies metálicas altamente dispersas, devido à sua estrutura porosa particular. Consequentemente uma pequena quantidade de metal introduzido na matriz zeolítica apresentará uma área superficial muito elevada, reduzindo desta forma a quantidade de metal necessário para obter resultados equivalentes aos que se verificam com os eléctrodos clássicos.

Os ensaios foram realizados numa célula de electrólise de Hoffman, estando ligados a esta uma fonte de tensão, um voltímetro e um amperímetro. Foi utilizado um zeólito do tipo BEA no qual foi introduzido um teor em metal de cerca de 1% por permuta iónica com uma solução aquosa de  $\text{Pt}(\text{NH}_3)_4\text{Cl}_2$ , seguida de calcinação e redução a 500°C sob fluxo de  $\text{H}_2$ . Ao zeólito com o metal disperso foi adicionada grafite que funciona como material condutor. A mistura, com uma

massa total de 250 mg foi então comprimida num pastilhador e adaptada a um suporte. Foi utilizado como electrólito uma solução aquosa de NaOH (10% p/v). Os ensaios foram realizados utilizando como eléctrodos pastilhas de grafite (G), grafite+zeólito (G+Z) e grafite+zeólito/Pt (G+Z/Pt). Para efeitos de comparação foram realizados ensaios utilizando eléctrodos de Pt. Em todos os ensaios foi aplicada na fonte de tensão uma d.d.p de 18 V. Com os resultados obtidos estabeleceu-se a seguinte sequência relativa às velocidades de formação de H<sub>2</sub> e O<sub>2</sub>:

$$\text{Pt} > (\text{G+Z/Pt}) > \text{G} > (\text{G+Z})$$

Os resultados permitiram demonstrar que pequenas quantidades de Pt introduzida no zeólito, em conjugação com a grafite apresentam um melhor desempenho electrolítico do que a utilização única de grafite. Estes mesmos eléctrodos têm um comportamento electrolítico ligeiramente inferior à platina. Os eléctrodos (G+Z) apresentaram o pior desempenho dado o carácter não condutor do zeólito. O estudo incidiu ainda sobre outros aspectos nomeadamente sobre a eficiência catódica e anódica, avaliada pela razão H<sub>2</sub>/O<sub>2</sub> para cada um dos materiais e sobre o comportamento mecânico e estabilidade dos eléctrodos ao longo do tempo.

# SOLUTION ENTHALPIES OF ADAMANTANE DERIVATIVES IN APROTIC SOLVENTS AT 298.15 K.

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Recent studies have shown that adamantyl compounds and their derivatives might have antibacterial and antiviral activity. One of the conditions to proceed with the use of any new compound for pharmaceutical purposes is the knowledge of its physicochemical characteristics. Solution calorimetry is in this context a powerful technique because it allows the identification of solute-solvent-solvent interaction mechanisms.

We have some published work on the solution enthalpies of 2-Br-2-methylpropane and 2-Br-2-methylbutane in hydroxylic solvents and more recently on the solution enthalpies of 1-bromoadamantane for the same set of solvents. These results show that the number and position of the OH groups, the length and branching of the alkyl chain of the alcohol and the size of the alkyl group of the solute determine the magnitude of the solution enthalpy.

In this work, we focused on the analysis of the effect of different functionalities in the infinite dilution enthalpies of solution,  $\Delta_s H^\infty$ , of a few adamantane derivatives in a set of aprotic solvents.  $\Delta_s H^\infty$  values at 298.15 K were determined with a precision solution calorimeter from Thermometric.

The thermochemical results were analyzed in terms of linear solvation energy relationships of the type  $\Delta_s H^\infty = f$  (solvent descriptors). The application of such an analysis, permitted the recognition of the dominant solute-solvent-solvent interaction mechanisms in the studied solution processes.

# INFLUENCE OF RARE EARTH ELEMENTS LA, ND AND YB ON PTBETA ZEOLITE FOR ISOMERIZATION OF N-HEXANE.

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HBeta zeolite with Si/Al ratio of 12.5 was submitted to ion exchanged with rare earth nitrate solutions of La, Nd and Yb followed by platinum introduction.

The influence of rare earth (RE) elements on the acidic properties of the catalysts was studied by pyridine adsorption followed by infrared spectroscopy and the model reaction of n-heptane cracking. The presence of two additional bands in the pyridine spectra and the raise in branched products with the simultaneous decrease in olefins are indicators that the presence of RE elements enhances the acidity of HBeta zeolite, especially YbBeta.

In the isomerization of n-hexane only PtYbBeta showed a slight decrease in total conversion, which was not affected by the number of ion exchanges for all RE elements. The major effect of RE introduction was in selectivity to di-branched products (2,2-DMB and 2,3DMB) that follows the sequence: PtNdBeta > PtLaBeta > PtYbBeta ≈ PtHBeta.

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2004.*

# ARGILAS COM PILARES DE ÓXIDOS DE Al, Zr e Al/Zr.

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Porto, Setembro de  
2004.*

Os resultados que se apresentam nesta comunicação integram-se num estudo mais alargado onde se pretende avaliar as potencialidades de argilas com pilares (PILCs), preparadas a partir de montmorilonites naturais portuguesas, como catalisadores de reacções pouco exigentes, em termos de acidez e temperatura, concretamente reacções de alquilação.

As PILCs estudadas foram obtidas a partir de uma montmorilonite natural proveniente de Benavila (Alentejo), caracterizada por um espaçamento basal de 1,50 nm e uma área específica de  $49 \text{ m}^2 \text{ g}^{-1}$ . As amostras com pilares de óxidos simples de Al e Zr preparam-se seguindo protocolos anteriormente estabelecidos. No que se refere à introdução de pilares mistos Al/Zr, a metodologia seguida consistiu em fazer intercalação da argila com uma solução de oligómero contendo Al e Zr. As amostras preparadas apresentam razões OH/Al=2 e metal/argila =  $11 \text{ mmol.g}^{-1}$ .

As amostras de PILCs foram caracterizadas por difracção de raios X e adsorção de  $\text{N}_2$  a baixa temperatura. Os dados de adsorção foram analisados através da aplicação das equações BET e Dubinin-Radushkevich de modo a estimar, respectivamente, a área específica e o volume microporoso das amostras.

Com o intuito de avaliar as potencialidades da amostras de PILCs como catalisadores ácidos foi efectuada sobre todos os sólidos a alquilação do tolueno pelo metanol. Constatou-se que todas as amostras mostraram propriedades alquilantes.

# ROLE OF SOLVENT VISCOSITY IN THE HETEROLYSIS REACTIONS OF TERTIARY ALKYL IODIDES. A NEW DYNAMIC APPROACH

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A current issue in solution phenomena is whether reactions occurring in condensed phases can still be described by a reaction coordinate or if a solvent coordinate must be included in order to correctly address this question<sup>1,2</sup>. Most of the designed studies have been performed on theoretical grounds and some made use of heterolysis reactions of tertiary alkyl halides<sup>3</sup>. The recognition of the influence of the solvent's motion on reactivity has been pointed out<sup>4</sup> and solvent's friction has become an interesting area of investigation. Still, the lack of relation between theoretical expressions involving friction and experimental work is one of the most challenging issues in dynamic reactivity studies<sup>5</sup>. With this work we aim to address these questions using a LSER's approach, involving the application of an extension of the TAKA's equation<sup>6</sup> which includes an extra solvent descriptor related to viscosity. We have measured log k values for three tertiary alkyl iodides in a set of protic and aprotic solvents. We show in this work an increase in the statistical confidence of the correlation between log k and several solvent descriptors, by including viscosity as a solvent property affecting reactivity. We claim that a correct interpretation of this fact leads to the experimental observation that a solvent coordinate also influences reactivity. A judicious choice of solvents, and therefore of descriptor's space, lead to an almost orthogonal training set of solvents. This allowed a quantification of the viscosity effect on reaction rates independently of all other effects in presence. This fact is a considerable improvement, as the interdependence among effects is one of the most common difficulties in these types of studies<sup>6</sup>.

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# SOLVENT EFFECTS ON THE HETEROLYSES REACTIONS OF TERTIARY ALKYL HALIDES. ROLE OF VISCOSITY IN REACTIVITY

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2004.

More than fifteen years have elapsed since Abraham et al.<sup>1</sup> published a paper on the comparative behaviour of t-BuX substrates (X = Cl, Br, I) in heterolyses reactions, based on solvent's contributions. At that time, the cohesive energy density was introduced as an explanatory variable, which represented an improvement regarding earlier work on the same subject.<sup>2</sup> Recently, we have expanded this study to similar, yet more crowded, substrates.<sup>3</sup>

The current work represents a comparison between six halogenated compounds varying in the carbonated frame and leaving group. We have measured log k values for the heterolyses reactions of 2-X-2-Methylpropane and 3-X-3-Methylpentane in an equal, diversified and balanced set of protic and aprotic solvents. Our results show, for some substrates, an increase in the statistical confidence of the correlation log k vs. solvent descriptors, when viscosity is included as a solvent property affecting reactivity, thus enlarging the scope of TAKA's equation.<sup>4</sup> We claim that this fact is an experimental evidence of the influence of the solvent coordinate upon reactivity, as already pointed out in solvation studies performed on theoretical grounds.<sup>5</sup>

# ALTERNATIVES TO Cr VI-BASED PRE-TREATMENTS FOR ALUMINIUM AND GALVANISED STEEL

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Cr-VI based pre-treatments have been in use for long time on several materials, namely on aluminium alloys and galvanised steels. As it is known health and environmental problems make them a target of great criticism and forthcoming legislation could definitely ban them. Different Cr-free alternatives have been reported, based on non-toxic or low toxicity chemicals, aiming at obtaining processes that confer to the treated surfaces corrosion resistance, adherence to organic coatings and fatigue resistance identical to those obtained with chromates.

The present study focus in some of the existing alternatives: organosilanes and hybrid sol-gel coatings. The organosilane used was Bis-[Triethoxysilylpropyl]Tetra-sulphide (BTESPT). The silane shows good affinity for Cu-containing substrates forming a homogeneous film on the AA2024-T3 alloys. For HDG two-step pre-treatments, involving the organosilane and rare earth salts (Ce, La) result in good corrosion protection. The use of hybrid sol-gel pre-treatments for aluminium alloy surface is a relatively new approach in corrosion protection and it is also considered. Sol-gel processes were initially explored for the deposition of inorganic oxide coatings, but in recent years the synthesis of organic-inorganic hybrid coatings acquire higher importance. The hybrid films show interest because they combine some properties from organic polymer materials and other properties from ceramic materials. The present investigation shows results of both the structure and the corrosion protective properties of nano structured sol-gel derived hybrid coatings on A2024-T3. The hybrid sols were prepared by copolymerization of 3-Glycidoxypropyltrimethoxysilane (GPTMS), tetraethylortosilicate (TEOS) and tetra-n-propoxyzirconium (TPOZ). The size of the incorporated ZrO<sub>2</sub> nanoparticles (from 20 to 200 nm) was regulated controlling the TPOZ hydrolysis time. It was found that the incorporation of the nanoparticles into the coating increases the corrosion performance of the hybrid pre-treatments.

The techniques used were d.c. polarisation, electrochemical impedance spectroscopy (EIS), SEM, atomic force microscopy associated with Kelvin probe (SKPFM), scanning vibrating electrode technique (SVET) and Auger/XPS spectroscopy. On painted specimens salt spray was

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carried out. The results obtained allow also discussing how certain species or films formed affect the rate of cathodic and anodic reactions and the barrier properties, i. e., the mechanisms involved in hindering corrosion.

# COMPUTER AIDED DETERMINATION OF OPTIMAL SUBSIDY FOR INSTALLING ENERGY SAVING EQUIPMENTS WITHIN AN INDUSTRIAL COMPLEX

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Utility plants supply the required energy demands to industrial processes, namely, mechanical, electrical and thermal power (different levels of steam). Several authors were addressed the synthesis and design of those plants. Among these authors, Oliveira Francisco and Matos (2003) described a multiperiod model for utility systems including environmental concerns by the application of the global emissions concept. The concept of global emissions accounts for the corrections to be made in local emissions due to increasing/decreasing external power plant emissions following power imports/exports by the local site. A superstructure for the utility plant was established. A Mixed Integer Linear Programming (MILP) formulation including restrictions for the global emissions (CO<sub>2</sub> and SO<sub>2</sub>) was implemented using the GAMS™ code. The model objective function includes the global emissions of gaseous pollutants as weighted terms. These weighted terms are a measure of the environmental impact due to the utility system, as expressed in monetary units.

The present paper describes a methodology for determination of optimal subsidy by the State of equipment providing energy saving and/or materials saving and/or environmental resources saving.

In order to apply the proposed methodology, the above referred MILP model for utility systems was solved for two situations: **a)** Synthesis and operational planning of a utility system without gas turbines.

**b)** State shall subsidy equipments (e.g., gas turbines) for reduction of environmental impact of the utility system.

The difference of environmental impacts in both situations corresponds to the environmental savings expressed in monetary units. This difference was taken as a basis for the determination of the subsidy (maximum for the investor, optimal for the State) as a function of several technical and economic parameters. The methodology adopted uses a combination of Return On Investment (ROI), after forecasting the pattern of cash flow, and break-even-point analysis.

A sensitivity study was performed by variation of (a) type and sulphur content of the fuel burned in the external power plant and (b) technical and economic parameter values within the corresponding intervals, as they were taken for two European countries (Portugal, Greece) and the EU as a whole.

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# SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF PIGMENTS FROM ANNATTO SEEDS (EXPERIMENTS AND MODELING).

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2004.*

Supercritical CO<sub>2</sub> extraction of pigments from annatto seeds was carried out at pressures of 200 bar and at temperature of 40 °C, in a flow apparatus, at two flow rates of fluid (0.67g/min and 1.12g/min). The efficiency of the extraction was low (about 1 % of the pigments were extracted). The increase in flow rate led to a decrease in extraction efficiency. A great increase in the yield (from 1% to 45%) was achieved using supercritical carbon dioxide, containing 5mol% of ethanol, as extraction fluid at pressures of 200 and 300 bar and temperatures of 40 and 60 °C. Although the temperature and the pressure led to an increase in yield, the changes in the flow rate seemed do not influence it. Furthermore, two unsteady plug flow models were applied to describe the supercritical extraction of the pigments from annatto seeds. Mass transfers coefficients were determined and compared with those obtained by other workers with similar models for the supercritical extraction of solutes from plant materials.

# PERFORMANCE EVALUATION OF TERTIARY TREATMENT OF WASTEWATER ON A LABORATORY-SCALE POND SYSTEM USING GRANULAR EXPANDED CLAY AS ATTACHED-GROWTH MEDIA

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The aim of this study was to investigate the potential usefulness of a natural material consisting of granular expanded clay (GrEC) to provide support for the growth of attached bacterial-algal biomass in attached-growth waste stabilization ponds (AGWSP) and to evaluate its effect on the performance of tertiary treatment. AGWSP is just a new-developed technology, about which there are a few studies reported in the literature, most of them consisting on experiences under laboratory or pilot-scale conditions and using artificial attached growth media (AGM). Based on the results of the laboratory experiments, we concluded a global improvement on the tertiary treatment due to the installation of GrEC as AGM in the reactors. Not only a significant increase in the total nitrogen and COD removal was observed, but we also noticed a strong reduction on the suspended algal biomass concentrations in the final effluent. The main mechanism causing improved nitrogen removal is hypothesized to be simultaneous nitrification/denitrification, which turned possible to remove both nitrate and ammonia from the effluent.

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*Proceedings da 6th INTERNATIONAL IWA CONFERENCE ON WASTE STABILISATION PONDS, Avignon, França, Set-Out de 2004.*

# MOLECULAR STRUCTURE AND CRYSTAL PACKING OF CpMR ISONITRILES (M = Ru, Fe; R = PHOSPHINES AND TMEDA). HOW TO OBTAIN NEW SOLIDS FOR NLO

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 M.F.M. da <sup>1,2</sup>; Dias, A.R.<sup>1</sup>; Duarte, M.T.<sup>1</sup>; Florindo, P.<sup>2</sup>;  
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Organometallic compounds have found great importance in the area of non linear optical materials, due to their significant values of second and third harmonic generation. This has been possible owing to the diversity of metal centres, oxidation states, ligands and geometries.

We present here a systematic study on Fe and Ru isonitrile derivatives, where we try to emphasize the relationship between molecular design and crystal engineering: the metal centers have been enriched and depleted by changing the type and number of ligands, the  $\pi$  systems have been extended and different counter ions have been used. The effects that this diversity has promoted in the 3D crystal packing will be discussed and compared.

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*5302.*

# INFLUÊNCIA DAS TERRAS RARAS LA, ND E YB NA ACIDEZ DOS ZEÓLITOS HMCM-22 E HBETA

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Nos zeólitos HMCM-22 e HBeta foram introduzidas terras raras por permuta iónica utilizando soluções de nitratos de La, Nd e Yb. A influência das terras raras (TR) nas propriedades ácidas dos zeólitos foi estudada usando a técnica de adsorção de piridina acompanhada por espectroscopia de Infravermelho (FTIR) e a reacção modelo de cracking do n-heptano.

Os espectros de infravermelho de TR-HMCM-22 indicam a presença dos catiões de TR nas supercavidades do zeólito e nos canais sinusoidais. Após adsorção da piridina, para além das bandas características dos centros ácidos de Brønsted e Lewis, detectam-se em TR-HMCM-22 e TR-HBeta a presença de duas bandas adicionais relativas à adsorção de piridina nos catiões TR<sup>3+</sup>.

A reacção de cracking do n-heptano mostra que o efeito da introdução de terras raras está directamente relacionado com o diâmetro e estrutura dos poros dos catalisadores. No zeólito HBeta a introdução das terras raras acentua as propriedades ácidas das amostras. No zeólito HMCM-22 a introdução dos catiões TR<sup>3+</sup> revela um efeito de selectividade de forma que se torna mais pronunciado com o aumento do raio iónico dos catiões.

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Simposio  
Iberoamericano de  
Catálisis, Mérida,  
Yucatán, México,  
Setembro 2004*

# ANÁLISE DO CONSUMO DE ENERGIA NA INDÚSTRIA PORTUGUESA, NA DÉCADA DE 90

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A melhoria de eficiência energética na produção de bens e serviços, entendida como a capacidade de produzir bens e serviços com menor consumo de energia, é um dos meios mais eficazes de controlo dos gases com efeito de estufa. O indicador mais correntemente utilizado para medir a eficiência na utilização do factor produtivo “energia” pelas economias é a intensidade energética do Produto Interno Bruto, ou seja a razão entre o consumo de energia final de determinado sector (ou do conjunto da economia) e o valor da produção desse sector (ou economia).

Desde o primeiro choque petrolífero que os países da OCDE têm vindo a reduzir a sua intensidade energética do produto, de tal modo que ao nível da OCDE o consumo de energia primária para produzir uma unidade de produto interno bruto diminuiu cerca de um terço desde 1973. No entanto esta evolução teve dinâmicas diferentes nos vários países da OCDE.

Portugal é um país usualmente apontado como tendo tido uma evolução menos dinâmica, e por vezes mesmo oposta, à evolução da intensidade energética do produto interno bruto na média da OCDE e da UE. Ou seja, enquanto na generalidade dos países a intensidade energética do PIB se tem reduzido significativamente, em Portugal ela tem aumentado, traduzindo a ideia que de em Portugal é necessário cada vez mais energia para produzir uma unidade de valor acrescentado. No entanto esta realidade carece de uma análise mais detalhada que tenha em conta os factores que determinam a evolução de indicadores muito agregados como a intensidade energética do PIB. Desde finais da década de 70 que foram desenvolvidas e utilizadas várias metodologias de análise da evolução do consumo de energia final. De um modo geral, essas metodologias assumem que o consumo de energia final de um sector ou sub-sector depende do seu nível de actividade (medido geralmente pelo VAB), da sua estrutura (medida pela importância relativa do contributo dos vários sub-sectores para o VAB do sector em análise) e da intensidade energética de cada sub-sector. Estas metodologias permitem assim decompor a evolução do consumo de energia final, nos vários efeitos que a determinam:

efeito de actividade, efeito de estrutura e efeito de eficiência. Ao invés de um indicador extremamente agregado e de leitura falaciosa, como é a intensidade energética do produto, é assim possível ter uma visão mais rica sobre a evolução do consumo de energia final e das suas determinantes e, por consequência, das determinantes das emissões de gases com efeito de estufa.

Nesta comunicação será feita uma análise para a indústria portuguesa baseada na metodologia Laspeyers e os resultados serão comparados com resultados de análises semelhantes para sectores industriais de outros países da OCDE e da UE, permitindo assim uma visão comparativa da evolução do consumo de energia na indústria. A análise cobrirá a última década do século passado, mas será apresentada conjuntamente com outros resultados obtidos pelos autores para a década de oitenta, o que permitirá ter uma visão global das determinantes do consumo de energia na indústria portuguesa nos últimos 20 anos que, como é conhecido, foi um período de profunda transformação do sector.

# DYNAMIC MOTION PLANNING FOR A SPRAY DRYER PLANT

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*Proceedings do  
Controlo 2004,  
Universidade do  
Algarve, Faro .*

This paper is concerned with motion planning between stationary states for moisture content in spray dryer plants. The problem consists in selecting the time profile of the manipulated variable (conveyor speed) such that the state (moisture level along the conveyor) is driven from one value to another as specified. The problem is solved by using the methods of flat systems and a change of the time variable such that the transformed system becomes flat.

# FLATNESS BASED ADAPTIVE TRACKING CONTROL FOR A DISTRIBUTED COLLECTOR SOLAR FIELD

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This paper is concerned with the design of an adaptive servo controller for tracking variable references in a distributed collector solar field. The structure proposed is made up of three main blocks: A motion planner, an incremental controller and an adaptation mechanism. The motion planner selects the time profile of the manipulated variable (oil flow) such that the plant state (oil temperature distribution along the solar field) is driven between successive equilibrium states as specified. This is done on the basis of a simplified, yet distributed parameter, model and uses the methods of flat systems and the concept of orbital flatness. In order to stabilize the actual oil temperature around this nominal path, a linear controller is used. This control law is then modified according to a Lyapunov function strategy for incorporating adaptation through the adjustment of a parameter which conveys the most significant plant uncertainty. The approach is illustrated through simulations performed in a detailed solar field model.

**Publicado em:**

*Proceedings do  
Mathematical Theory  
of Networks and  
Systems (MTNS),  
Katholieke Universiteit  
Leuven, Bélgica.*

# VARIABLE SAMPLING RATE OBSERVERS FOR STATE ESTIMATION IN DISTRIBUTED COLLECTOR SOLAR FIELDS

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This paper is concerned with state estimation in physical plants involving transport phenomena with no diffusion. These are described by an hyperbolic partial differential equation where the manipulated variable multiplies the state (bilinear structure). Distributed collector solar fields, where the state is the temperature distribution along the field, provide an example which is treated in detail. Observers of two types are considered. The first relies on the method of characteristics and the second on the orthogonal collocation method. A distinctive feature of the paper consists in the fact that both methods explore a change of time scale, which provides an exact linearization of the plant model. For discrete time approximations, this amounts to the use of a variable sampling interval. The stability of the observer filters is established. The observer algorithms are tested through simulations performed in a detailed physical model of the solar field.

**Publicado em:**

*Proceedings do 6th  
IFAC Symposium on  
Nonlinear Control  
(NOLCOS), Universität  
Stuttgart, Alemanha.*

# DYNAMIC MOTION PLANNING OF A DISTRIBUTED COLLECTOR SOLAR FIELD

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This paper is concerned with motion planning for distributed collector solar fields. The problem consists in selecting the time profile of the manipulated variable (oil flow) such that the state (temperature distribution along the field) is driven from one value to another as specified. The problem is solved by using the methods of flat systems and a change of the time variable. Two solutions are provided, one directly for the distributed parameter model and another for a lumped parameter model resulting from space sampling of the distributed model.

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*Proceedings do 6th IFAC Symposium on Nonlinear Control (NOLCOS), Universität Stuttgart, Alemanha.*

# POLÍMEROS FUNCIONAIS CONTENDO CALIXARENOS – SÍNTESE E APLICAÇÕES

**Barata, Patrícia Alexandra Miranda David**

**Mestrado em:** Química Orgânica Tecnológica

**Grau Concedido por:** FCT – Universidade Nova de Lisboa

**Orientadores:** José Virgílio Prata

**Provas Concluídas em:** 7 de Maio de 2004

Neste trabalho são descritas as sínteses de novos polímeros lineares e entrecruzados contendo unidades de calix[4,6,8]arenos com potencial aplicação em catálise e em processos de extracção selectiva. A preparação dos polímeros envolveu duas metodologias distintas. A primeira permitiu a ligação directa de *p-tert*-butilcalix[4,6,8]arenos e *O*-tripropil-*p-tert*-butilcalix[4]areno a resinas do tipo Merrifield originando, de modo simples e eficaz, polímeros com diversos graus de incorporação. A segunda envolveu a copolimerização de *O*-tripropil-*p-tert*-butilcalix[4]areno funcionalizado com unidade vinílica e estireno; o controlo do grau de incorporação e do grau de entrecruzamento permitiu a obtenção de polímeros lineares (eg.  $T_g = 120^{\circ}\text{C}$ ;  $M_w = 41000 \text{ gmol}^{-1}$ ) e entrecruzados ( $T_g = 141^{\circ}\text{C}$ ), com graus de conversão de 51-61%. Em ambos os métodos a ligação ocorreu via coroa inferior do macrociclo. Alguns dos polímeros obtidos foram posteriormente modificados através da introdução de grupos hidrofílicos na unidade de calixareno. A capacidade de sorção dos polímeros sintetizados face a espécies fenólicas presentes em solução aquosa foi avaliada através de estudos de sorção; a escolha de moléculas de sonda (fenol, 2,4-diclorofenol e  $\beta$ -naftol) com níveis de acidez e hidrofília diferenciados permitiu correlacionar estes parâmetros com a capacidade de sorção. Foi observada maior eficiência na extracção com polímeros contendo unidades de calixarenos com derivados carboxilatos.



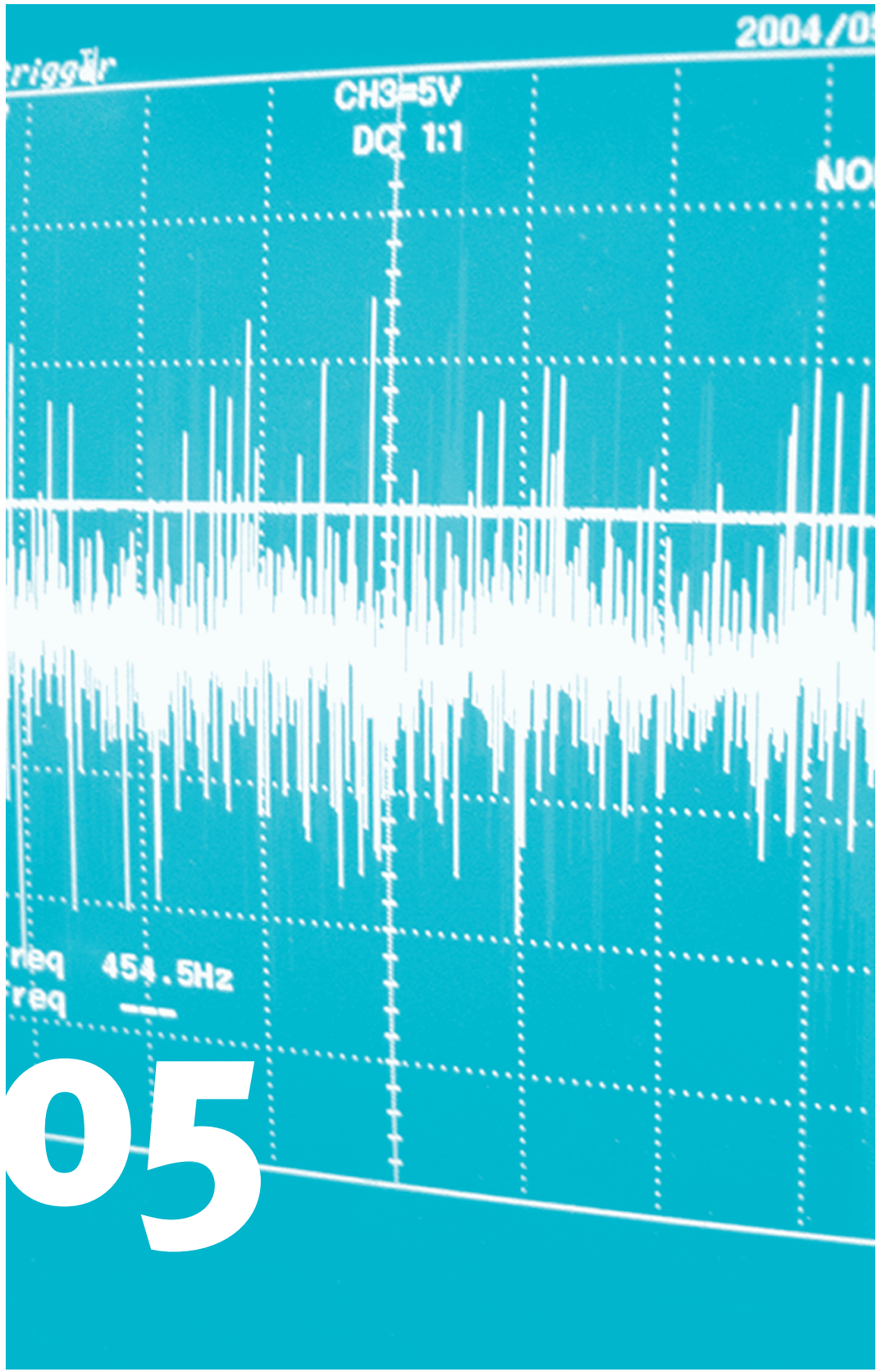
Trigger

CH3=5V  
DC 1:1

NO

req 454.5Hz  
req

# 05



# ENGENHARIA DE SISTEMAS DE POTÊNCIA E AUTOMAÇÃO

Anuário Científico 2004

ISEL



# NUEVO MÉTODO PARA LA SIMULACIÓN DEL MODELO ELECTROGEOMÉTRICO UTILIZANDO EL AUTOCAD

**Rodrigues, Rafael; Soares, Constantino V.**

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El objetivo principal del trabajo presentado aquí fue el desarrollo de un programa de ordenador, el SPDA 2002, para simular el modelo electrogeométrico. El programa también permite el análisis del riesgo a que un edificio o conjunto de edificios están sujetos, según las normas BS 6651 y IEC 61662. Se utiliza el AutoCAD®, como herramienta de dibujo por ordenador, para modelar en 3D los edificios a proteger. El SPDA 2002 nos permite conocer la eficiencia necesaria del pararrayos y así simular el modelo electrogeométrico con el nivel de protección más adecuado. De esta simulación resulta, automáticamente, un dibujo 3D con todos los puntos vulnerables señalados. Resultan además otras indicaciones útiles para la protección contra los efectos indirectos de las descargas atmosféricas. De la utilización del SPDA 2002 se observó una importante reducción del tiempo necesario, en la concepción de un sistema de protección contra los efectos de las descargas atmosféricas.

**Publicado em:**

*La revista internacional "Información Tecnológica" (ISSN: 0716-8576), Chile, Fevereiro de 2004*

# ELECTRICAL MOTORIZED WHEEL MOTOR DESIGN

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Lisboa, Portugal

In this paper a special purpose designed electric motor for the Electric Motorized (EM) wheel is presented.

By describing the evolution of the wheel into a motorized one focusing in the EM one, an overview of the state of art this approach is given. Using as a starting point the definition of the desired characteristics of an electrical motor for the EM wheel, the special purpose compact permanent magnet electrical machine was designed to be the applied into several Electrical Vehicle (EV) platforms.

Electromagnetic analyses of the proposed machine are performed with analytical calculations and by using finite element methods, including torque ripple and eddy current calculations.

The industrial applicability of the proposed machine is also used to characterize the current trends in the field.

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*Actas da Conferência  
Europeia ELE-DRIVE  
TRANSPORTATION,  
March 2004.*

# EVALUATION PROCEDURE FOR ALTERNATIVE PROPULSION DRIVETRAINS: APLICATION TO A POSTAL SERVICE FLEET

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The search for alternative propulsion solutions has been intensive and the companies that depend on mobility for their activities are investing on those alternative solutions to be prepared for the future.

CTT, Correios de Portugal, is the major company working on the activity of Postal services in Portugal with a 3426 vehicles fleet. After a four years experience on the introduction of four electric Citroen Berlingo in urban postal distribution, the company wants to continue the introduction of alternative propulsion vehicles in the segment of small vans representing 26,7 % of the fleet.

For the segment of small vans the alternative propulsion vehicles available at the Portuguese market are only two. One is an Electrical Vehicle (EV), the Citroen Berlingo already tested; the other is a Compressed Natural Gas Vehicle (CNGV), a Fiat Doblo. Their performance and pollutant gaseous emissions must be compared with their direct established competitors, Diesel small vans proposed by the different manufacturers.

A comparison and evaluation procedure for the different alternative propulsion drivetrains is developed in this paper.

As the comparison and evaluation process involves several aspects at same time, it is proposed to use a simulation tool, ADVISOR, in order to evaluate the different drivetrains performances. The use of this simulation tool allows a vehicle model construction and to run several simulations over different conditions.

## **Publicado em:**

*Book of Abstracts,  
2004 European Ele-  
Drive Transportation  
Conference and  
Exhibition, Estoril,  
Portugal, March 2004*

# POSTAL DISTRIBUTION WITH EV'S IN PORTUGAL

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 Drive Transportation  
 Conference and  
 Exhibition, Estoril,  
 Portugal, March 2004*

This paper describes the experience of the Portuguese Post with electric vehicles for Postal Delivery.

In 1999, the Portuguese Post, CTT, acquired two Citroën Berlingo Electric to be used for postal delivery in the city of Évora. This was the first experiment with electric vehicles in the Portuguese Post and included an extensive program of monitoring, to evaluate the energy, environmental and economical performance of this type of vehicles. Among other parameters, the monitoring included the measurement of energy consumption, distance travelled and cost of energy, which enabled the calculation of relevant indicators, such as consumption of energy according to the distance or the operational cost of these vehicles. The results of this experiment enabled the evaluation of the potential for the use of electric vehicles in the fleet of the Portuguese Post, which has been a tool to justify the acquisition of two more Citroën Berlingo Electric, that are being used in the cities of Aveiro and Ponte de Lima.

The measured range of the four vehicles varies between 40 km, for vehicles operating since 1999, and 60 km, for the more recent.

The opinions of the drivers and population are globally very positive. The absence of noise, pollutant emissions and the relaxed driving that they provide are pointed as the main advantages of these vehicles.

A brief economical analysis shows that the operational costs of the electric vehicles are roughly 1/3 of the costs of a conventional (Diesel) vehicle performing the same task.

# USING A HYBRID EVOLUTIONARY-TABOO ALGORITHM TO SOLVE JOB SHOP PROBLEM.

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Rosa, Agostinho C.<sup>3</sup>

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- 3 LaSEEB-ISR-IST, Lisboa, Portugal

In this paper, we propose a new hybrid algorithm to solve the Job Shop Problem. Our algorithm, called Evolutionary-Taboo uses an Evolutionary Algorithm (EA) to enhance results obtained by one of the best Taboo algorithms for this problem. We tested the algorithm on the benchmark problems for which the taboo algorithm returned its worst results. On average, we improved taboo results by 2.9%. Final results were under one percent from the best know results for these problems.

**Publicado em:**

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19th Annual ACM  
Symposium on  
Applied Computing,  
ACM SAC'04, Nicosia,  
Chipre, Março 2004.*

# CONTRIBUTION TO A CONCEPTUAL BASIS FOR THE STUDY OF POWER ELECTRONICS CONVERTER TOPOLOGIES

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Conference on  
Innovation in  
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and Information  
Engineering, Sofia,  
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A power electronics circuit consists essentially of an array of semiconductor switches placed between two adjacent circuits. This principle is well known and mentioned in every textbook; however, a truly systematic deduction or synthesis of existing converter topologies, based on switches and valve elements, is not provided. Such an attempt is presented in this paper.

Elementary structures are initially established by starting with two-port switch circuits, and taking into account the most stringent boundary conditions; the role of the valve function is then introduced. Elementary structures suitable for uni-directionally (i.e. DC) impressed voltage and current are associated with the purpose of creating topologies suitable for bi-directional (i.e. AC) quantities. Then new association and generalisation steps are used with explicit objectives leading to a number of DC-DC, AC-DC and AC-AC structures covering a wide group of well known converter families. Specific switch-valve arrangements required for each class of converters (rectifiers, inverters, direct frequency changers) appear naturally as a by-product of the deductive process.

Comments on teaching methodology and converters classification conclude the study.

# ELECTRICITY MARKETS SIMULATION - AN APPLICATION TO THE IBERIAN ELECTRICITY MARKET - MIBEL

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A liberalized market is a market where customers can freely choose their supplier. This market model came with the introduction of competition into non-competitive regulated markets. In a non-competitive environment, supply and prices are regulated, while in a liberalized market regulation aims at avoiding the abuse of market power. In the case of electricity, the starting point was the rigorous analysis of the sectors of the industry which were natural monopolies and the identification of the activities where the barriers to entry were such that no competition will develop naturally. It had been assumed in former market organization that the whole of the electricity industry was a natural monopoly which led to the acceptance of vertically integrated monopoly supply utilities. On a closer inspection it was found that only certain activities were natural monopolies, in particular the transmission and distribution networks. This discovery led reformers to search for mechanisms of introducing competition wherever this seemed possible. Bearing in mind the upcoming Iberian Electricity Market – MIBEL, we studied the sensitivity of the Market Clearing Price to changes in the production inputs, such as coal, natural gas and fuel. Parallel to the privatization process of electricity utilities and the liberalization of the European electricity markets, the Portuguese and Spanish markets engaged in a process of integration which will lead to the upcoming Iberian Electricity Market (MIBEL). In both countries it has been introduced changes in the production, transmission and distribution of electricity sectors with the aim of achieving a legally, socially and economically unified market.

**Publicado em:**

*Actas ENERGEX – 10th  
International Energy  
Forum 2004 | Energy  
& Society: 3–6 May  
2004, Lisbon, Portugal*

# DYNAMIC MODELLING OF WIND TURBINE

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**2** Departamento de Engenharia Electrotécnica e Automação, ISEL, Lisboa, Portugal

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International  
Conference ENERGY &  
SOCIETY, Lisbon,  
Portugal, May 3-6,  
2004.*

This paper is on the wind energy use for power systems plants with a focus on the dynamic modelling of a wind turbine.

The growths of energy conversion should be oriented in a way to decrease the dependency from fossil fuels. Simultaneously, it is absolutely indispensable to provide the required energy taking into account the constraints related to a clean environment.

Hence, an unprecedented change points to a scenario where renewable energy sources will be a significant component of the total generation mix. Wind power plants electric capacity in Portugal is presented and a study of a horizontal axis wind turbine concerning the blades pitch angle control is illustrated.

# HYDROELECTRIC ENERGY: ON SHORT-TERM OPERATION SCHEDULE

**Mendes, V.M.F.<sup>1</sup>; Catalão, J.P.S.<sup>2</sup>;  
Mariano, S.J.P.S.<sup>2</sup>; Ferreira, L.A.F.M.<sup>3</sup>**

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Universidade da Beira Interior, Covilhã, Portugal

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This paper is on hydroelectric energy and particularly is on the assessment of the accurate short-run managing decision for the electric energy, article of trade, on nowadays energy market.

We present the main features for this article of trade and for hydro energy resources in what regards managing, particularly, in the short run known as short-term operation schedule problem.

We point out as challenge to this problem to combine engineering management knowledge of hydroelectric energy resources with computer simulation methods to improve the support for achieving the best decisions.

Finally, we present as a case study a short-term operation schedule to handle head-sensitive reservoirs based on a non-linear network programming problem approach.

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Portugal, May 3-6,  
2004.*

# ENERGY EDUCATION: ON EMISSION CONSTRAINTS

**Mousinho, Jorge; Mendes, V.M.F.**

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**Publicado em:**  
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International  
Conference ENERGY &  
SOCIETY, Lisbon,  
Portugal, May 3-6,  
2004.*

This paper is on damage of our environment resulting from human activities particularly we access the pollution emission coming from electric energy power plants burning coal, oil, or gas to convert into electric energy. Education on power systems environmental pollutant emission constraints is important for preparing the future engineers to deal with this issue. We present an approach concerning the teaching of emission constraints on short-term power systems scheduling and economical dispatch.

Power systems companies with old coal-fired power plants technology in used two decades ago have higher levels of pollution. Although, with the actual technology coal-fired power plants are polluting less, if they are in the vicinity of urban or rural zones, then concentration of pollution can originate environmental impact.

Electric power sector deregulation brought to the electric power business competitions through bidding to win the best profit in the electric energy market. The electric energy conversion should be responsible for the pollutant emissions, taking into account constraints to ensure admissible levels of emissions in the environment. The paper is structured as follows. The emission bounds section provides a preamble concerning the emission protocol of Kyoto, presenting total carbon dioxide equivalent emission granted and the reduction commitment. The fuel: coal, oil, gas section provides an overview of the fuels used on electric energy utilities. The notation section describes the symbols used throughout this paper. The emission constraints formulation section provides a formulation for short-term scheduling of utilities considering emission constraints. Finally, we present a case study.

# REGULATION AND DEREGULATION: ON COMPENSATION FOR ENERGY NOT SUPPLIED

**Domingues, Nuno<sup>1</sup>; Gomes, Tiago<sup>1</sup>;  
Metz, Dieter<sup>2</sup>; Mendes, Victor<sup>2</sup>**

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**2** F.D., Fachhochschule Darmstadt-University of Applied Science,  
Germany

Usually power system engineers are trained to take care of the technical part of the power system, but nowadays skills merging technical and economic knowledge are needed. Electric power markets are changing rapidly. Also, new players appear in the electricity business. The principal drivers of change include privatisation, market liberalization and regulatory reform. The implementation of electric power markets differs from country to country and there is still an actual change in the political, legal, economical and technical fields of several countries. The economic decisions of utility management have got a high significance in a way of forcing to reduce costs. All divisions of the companies and all tasks have to match economic constrains because the prices are under market rules. Due to this philosophy, a strong pressure to lower the staff labour costs came out, technical investments have been seriously reduced and the investment on maintenance was decreased. However, if failures or even emergency situations occur, they directly influence quality of power system supply. Hence, they influence the customers' feelings.

Operation strategies are expected to be more effective when taking account the economic constraints, like penalty financial Compensations for Energy Not Supplied (CENS) to be paid to customers. We studied regulation's penalties in different countries to keep good quality of the energy supply. We developed an application to compute the CENS in an implemented SCADA system. We present a case study using our application, showing how to improve technical skills based on economic indicators. Obviously, additional benefits can be expected by using optimised operational strategies. Results of a market survey clearly indicate that additional benefits are achieved.

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International  
Conference ENERGY &  
SOCIETY, Lisbon,  
Portugal, May 3-6,  
2004.*

# ON POWER SYSTEMS EMISSION CONSTRAINTS

**Mendes, V.M.F.<sup>1</sup>; Mariano, S.J.P.S.<sup>2</sup>;  
Catalão, J.P.S.<sup>3</sup>; Ferreira, L.A.F.M.<sup>3</sup>**

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The power electricity systems sector has change from vertically integration, covering conversion, transmission, distribution and supply of electric energy in state owned monopolistic companies to competition in wholesale markets, awarding customers to choose suppliers.

Nowadays within liberalized energy power markets a power system can be viewed as a set of companies intended for forms of energy conversion into electric energy.

The management decisions of those companies are derived by profitable bid submitted to the market, supporting those decisions is usually a guess for the anticipated energy future prices. Some of those companies are environmental affecting our habitat more than others, that is, they are an important source of pollution when compared with others.

Emission constraints have to become an increasing issue to be considered in the management of the electric companies. Consequently, developing an education curriculum merging technical and economic knowledge with concerns on emission constraints for schedule of thermal units burning fossil fuel is imperative for the future engineers to face the proper decisions.

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Innovation in  
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and Information  
Engineering (EAEEIE  
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2004, Sofia, Bulgaria*

# SCHEDULING OF HEAD-SENSITIVE CASCADED HYDRO SYSTEMS: A COMPARISON BASED ON NUMERICAL SIMULATION RESULTS

Catalão, J.P.S.<sup>1</sup>; Mariano, S.J.P.S.<sup>1</sup>;  
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In the present day, with the deregulation of the electric power sector, business is recognized as a bid to win the best profit. In this new and competitive environment, a hydroelectric power utility has to decide the optimal management of the inflows and the water stored in its reservoirs, maximizing profit from selling energy without compromising future potential profit. This paper is on the problem of short-term hydro scheduling, concerning head-sensitive cascaded reservoirs, and the algorithmic aspects of its solution. We propose and compare optimization methods based on dynamic programming, linear and non-linear network programming. Finally, based on numerical simulation results, we report and illustrate our experience.

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Conference on Power  
and Energy Systems  
(EuroPES 2004):  
28-30, June, 2004,  
Rhodes, Greece*

# DECOUPLING OF AN EV ACTIVE STEERING AND DIRECT YAW MOMENT CONTROL SYSTEMS

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By considering a four-wheel-motor EV, the present paper addresses the EV stabilization using the advantages of electrical motorized wheels incorporation. The decoupling of the control of the active steering control (AFS) and the direct yaw moment control (DYC) as a way of controlling the vehicle's body slip angle and its yaw rate simultaneously, also allows the stabilization of the lateral motion of the EV.

**Publicado em:**

*WSEAS  
TRANSACTIONS on  
MATHEMATICS, Issue  
3, Volume 3  
ISSN: 1109-2769, July  
2004.*

# NEW APPROACH TO CONTROL SRM DRIVES

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This paper presents a new approach to the control of the turn-on angle used to excite the switched reluctance motor (SRM). The control algorithm determines the turn-on angle that supports the most efficient operation of the motor drive system, and can be divided in two fractions. One fraction of the control algorithm monitors the position of the first peak of the phase current ( $\theta_p$ ) and seeks to align this position with the angle where the inductance begins to increase ( $\theta_m$ ). The second fraction of the controller algorithm monitors the peak phase current and advances the turn-on angle if the commanded reference current cannot be produced by the controller. The first fraction of the controller tends to be active below nominal speed of the SRM, where phase currents can be built easily by the inverter and  $\theta_p$  is relatively independent of  $\theta_m$ . The second fraction of the controller is active above nominal speed, where the peak of the phase currents tends to naturally occur at  $\theta_m$  regardless of the current amplitude. Simulation and experimental results prove that this algorithm provides an efficient operation of the SRM drive.

**Publicado em:**  
*WSEAS TRANSACTIONS  
on SYSTEM, Issue 5,  
Volume 3  
ISSN: 1109-2777, July  
2004.*

# PHOTOVOLTAIC TECHNOLOGY AND THE REGIONAL DEVELOPMENT

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Large Photovoltaic power systems can be key factors for regional development. Countries in South of Europe have annually a great number of hours of Sun with good conditions to produce electricity with photovoltaic (PV) systems.

In those regions, large PV power plants can generate more added values to regional development, other than the production and commercialization of electricity. This paper presents an analysis of one case-study located in south of Portugal, calculating the annual energy and evaluates different incentive scenarios and corresponding results. At the end, presents different proposals for government incentives to accelerate the use of photovoltaic installations.

**Publicado em:**

*WSEAS TRANSACTIONS  
on CIRCUITS and  
SYSTEMS  
Issue 6, Volume 3  
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August 2004*

# TWO NEIGHBOURHOOD APPROACHES TO THE TIMETABLING PROBLEM

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It is well known that any search algorithm needs for certain parts to be problem specific. It is very important the way these parts are implemented. A fine tuning of parameters will never balance a bad definition of the solution set, of the neighbourhood or the cost function. In this paper we try to compare two well known neighbourhood operators applied to the timetabling problem. Tests were made using real data from three Portuguese schools of different size and complexity. We then observed that the application of the correct neighbourhood operator is essential to the success of the search algorithm.

**Publicado em:**  
*Proceedings of The  
5th International  
Conference on the  
Practice and Theory of  
Automated  
Timetabling,  
Pittsburgh, USA,  
Agosto 2004.*

# EMISSION CONSTRAINTS ON SHORT-TERM SCHEDULE OF THERMAL UNITS

**Mendes, V.M.F.<sup>1</sup>; Mariano, S.J.P.S.<sup>2</sup>; Catalão, J.P.S.<sup>1</sup>; Ferreira, L.A.F.M.<sup>3</sup>**

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This paper is about environmental protection of our habitat in what regards limiting the pollutant emission due to thermal power plants, burning fossil fuels, burning coal, oil and gas to convert into electric energy.

In one hand, within the liberalized energy power markets, schedule of thermal power plants has dislodged from electric companies point of view optimisation problem to a market level problem.

In another hand, as a consequence of growing environmental concern, the impact of conventional power plants, on the environment is being considered and efforts are being made to limit this impact.

Hence, the short-term schedule for thermal power plants needs to be not only considered within the market, but also in a way with acceptable pollutant emissions in the environment.

We present a case study for thermal power plants considering pollutant emissions and compare the results with the usual non-emission approach.

**Publicado em:**

*Proceedings of the  
39th International  
Universities Power  
Engineering  
Conference (UPEC  
2004):06-08  
September, 2004,  
Bristol, United  
Kingdom.*

# DRIFT ANGLE OBSERVER DESIGN FOR VEHICLE CONTROL

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- 3 APVE, Lisboa, Portugal

In the present paper the problem of the vehicle's body slip angle increase, leading to a dangerous driving situation, is addressed. To reduce this potential problem the proposed solution relies on maintaining a small value of the body slip angle. Since an expensive optical sensor is required to measure it, the present paper proposes to estimate it accurately with a simple linear observer, which is robust to the model variation and works well even in non-linear region of vehicle motion. To validate the proposed observer behaviour, numerical simulations and some results based on experimental data are shown.

**Publicado em:**

*WSEAS Transactions  
on Systems, Issue 7,  
Volume 3, Turkey,  
September 2004.  
ISSN: 1109-2777, 13-16  
September 2004*

# INDUCTION GENERATOR EXCITED BY VOLTAGE SOURCE INVERTER FOR MICRO-HYDRIC PLANTS.

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**Publicado em:**  
*Actas da XVI  
International  
Conference on Electric  
Machines, Cracow-  
Polónia, Setembro de  
2004*

The trend to reduce dependency of pollutant energetic sources has been increasing in developed societies. Therefore, there is a growing interest in the exploitation of small renewable energetic resources such as micro-hydro sources. In low power micro-hydro plants (< 50kW), the use of induction generators have been gaining significant importance relatively to other types of generators, due to its robustness, reduced costs and low maintenance. However, the main disadvantage is related to the needing of an exterior source to supply reactive power. Hence, the application of a static power converter, as a reactive source, presents itself a good solution. With the proper control strategy, this static VAR system, can provide an efficient excitation to the generator, as well as the possibility of continuous regulation in a large range of speed and load variation.

# MODELLING POWER PLANTS EMISSION CONSTRAINTS

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This paper is on damage due to human activities on our environment in the context of measures against environment pollution. More precisely, we access the pollution emission coming from electric energy power plants burning coal, oil, or gas to convert into electric energy. Power systems emission constraints are important for dealing with the limitation on pollutant emissions, as a result of the international community concern, expressed at diverse world encounters in response to the increase of pollution in our environment due to the use of the conventional fossil fuels. We present a modelling approach concerning the power plant emission constraints and a case study for a static scheduling of thermal units.

Environmentalists have claimed that change in the global environment in the last century due to emissions pollution has been a major force in our climate. Protection against degradation of our environment still is an unsolved issue, but significant steps are moving in the right direction. The paper is structured as follows. The constraints on emissions section provide a preamble concerning the emission protocol of Kyoto. The fossil fuel section provides an overview of the fuels used on electric energy utilities. The notation section describes the symbols used throughout this paper. The problem formulation section provides a formulation for short-term scheduling of utilities considering emission constraints. Finally, the case study section presents a case study for a static schedule of thermal units, considering emission constraints.

**Publicado em:**

*WSEAS Transactions on Systems, Issue 7, Volume 3, Turkey, September 2004.*

# STABILITY MODELLING OF WECS FOR POWER GENERATION

**Fonte, Pedro; Quadrado, José Carlos**

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Lisboa, Portugal

**Publicado em:**  
*WSEAS TRANSACTIONS*  
on *CIRCUITS and*  
*SYSTEMS*, Issue 7,  
Volume 3  
ISSN: 1109-2734,  
September 2004.

Several new generation and storage technologies have the potential to significantly impact power system performance. Some of these new technologies are well suited for distributed generation and storage applications. The purpose of this brochure is to define the characteristics of various new forms of generation and storage salient to studies of power system dynamics in the transient stability range and slower. This type of characterization is the first step in developing models and simulation methods appropriate for studying power system dynamics and the effects of introducing new forms of generation. Wind energy conversion systems, small hydro turbines, micro-turbines, fuel cells, photovoltaic systems, superconducting magnetic energy storage systems, battery energy storage systems and flywheels are mainly addressed in this paper.

# TEACHING OVERVOLTAGE PROTECTION ON LOW VOLTAGE AND TELECOMMUNICATION SYSTEMS BASED ON INTERNATIONAL STANDARDS

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This work proposes a computer program – the SPST 2003 – useful to evaluate the risk of damages, on telecommunication lines, due to lightning and overvoltages. Based on IEC 61663-1, IEC 61663-2 and AutoCAD 2004®, the SPST 2003 was developed as an educational tool to be used on teaching the risk of damage on telecommunication lines, either for cables with fiber optics or metallic conductors. This software also helps the designer on establish the adequate protection system. Because analysis of risk of damage on buildings requires specific standards, an automatic link to other software is established when necessary. Students get acquaintance and knowledge by using SPST 2003 and can solve practical problems saving time.

**Publicado em:**

*Actas da “11th International Power Electronics and Motion Control Conference – EPE PEMC”, Riga, Letónia, Setembro de 2004.*

# CONVERTER TOPOLOGY SELECTION FOR FC-HEV

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Lisboa, Portugal

In future hybrid electric vehicles (HEV), high-power DC/DC converters are used to connect fuel cells or high-voltage batteries with the motor drive. Several fuel cell system architectures for HEVs were studied. The most promising architecture only needs one bi-directional DC/DC converter. In this paper, a comparison of different bi-directional DC/DC converter topologies is presented. The goal is to find a topology which is suitable for this application and fulfils the given requirements.

**Publicado em:**

*WSEAS TRANSACTIONS  
on CIRCUITS and  
SYSTEMS, Issue 8,  
Volume 3  
ISSN: 1109-2734,  
October 2004.*

# HYBRID PV-FC POWER SYSTEM

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The purpose of the work is to design and optimise the operation of a system coupling a photovoltaic field, an electrolyser, a gas storage unit, a fuel cell and a power management unit using the cutting-edge technology materials. Such a hybrid system is intended to be an environmentally friendly solution, to maximise the use of the renewable energy production and in a near future to decrease the current level of investment and running costs. All components have been selected for an optimal, automatic, safe and reliable operation of the complete system. Fully instrumented, this test bench aims to furnish new data concerning each component and the complete system behaviour for variable real weather conditions and different load demands. The paper will present the complete description of the intended PV-FC system. It will point out the most important advantages and the competitive forecasted prices of that kind of systems.

**Publicado em:**  
*WSEAS TRANSACTIONS  
on CIRCUITS and  
SYSTEMS  
Issue 8, Volume 3  
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October 2004*

# IMPACTO DO COMÉRCIO DE EMISSÕES DE CO<sub>2</sub> NO SECTOR ELÉCTRICO: UMA APLICAÇÃO AO MIBEL

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**Publicado em:**

*IST Forum Energia  
– Outono 04, IST,  
Lisboa, Portugal,  
Novembro 2004.*

As emissões de gases com efeito de estufa (GEE) resultante da actividade humana, denominadas emissões antropogénicas, têm merecido especial atenção por parte da comunidade internacional devido às consequências que colocam ao nível do aquecimento global do planeta. Com vista ao estabelecimento de medidas que minimizem este problema foram criadas diversas instâncias internacionais de debate, tendo-se estabelecido, em Dezembro de 1997, o Protocolo de Quioto. O Protocolo obriga a União Europeia (UE) e os seus Estados-membros a reduzirem as suas emissões antropogénicas agregadas de GEE em 8 %, relativamente aos níveis de 1990, no período de 2008 a 2012. Os limites de emissão foram estabelecidos para cada um dos Estados-membros de acordo com as suas especificidades, tendo Portugal um objectivo de aumento máximo de 27% e Espanha um aumento máximo de 15%. No Protocolo estão previstos três mecanismos de flexibilidade que permitem alcançar os objectivos estabelecidos de forma economicamente eficiente: o Comércio de Emissões (CE), a Implementação Conjunta (IC) e o Mecanismo de Desenvolvimento Limpo (MDL). Atendendo à progressiva integração do mercado português e espanhol, a avaliação do impacto do Comércio de Emissões foi realizada ao nível do MIBEL - Mercado Ibérico de Electricidade em contexto de internalização dos custos de emissão de CO<sub>2</sub>. Para o efeito foi desenvolvido um simulador denominado SIMEC - Simulador do Mercado Eléctrico e do Carbono, que determina o preço de fecho do mercado de energia eléctrica, a produção de energia eléctrica por central, o nível de emissões de CO<sub>2</sub> por central e o lucro de cada empresa produtora.

# LINEAR CONTROLLER FOR MAGLEV MOTOR WITH AXIAL FLUX

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Lisboa, Portugal

In this paper, in order to stimulate the development of active bearings (AMB) systems we propose a linear controller design for maglev motors, based on forces and voltages required for stable control of the rotor in the radial direction. The control currents intentionally break force symmetry, resulting in unbalanced radial forces. The system employs two stators to effectively remove the rotational frequency modulation effect in the radial control forces.

**Publicado em:**  
*WSEAS Transactions  
on Circuits and  
Systems, Issue 9,  
Volume 3, November  
2004.*

# MODELIZAÇÃO E CALIBRAÇÃO AUTOMÁTICA DE TERMOPARES

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**Publicado em:**  
 1<sup>o</sup> Encontro Nacional  
 da Sociedade  
 Portuguesa de  
 Metrologia, IPQ,  
 Portugal, Novembro  
 de 2004.

Apresenta-se um programa para calibração automática de termopares, quer para valores discretos quer para valores contínuos, numa dada gama de temperatura. Para os dois modos de calibração são indicados as correspondentes estimativas da incerteza combinada.

O modelo de variável única, do tipo constante mais erro  $y = C + \varepsilon$ , é o ponto de partida do método de medida utilizado. Para que este modelo possa ser aplicado são verificadas experimentalmente as quatro condições fundamentais que garantem a sua validade: média e variabilidade constantes, aleatoriedade e distribuição normal fixa.

Com base nestas condições são definidos os critérios para aquisição automática de dados de temperatura e, particularmente, o número de aquisições e respectivo espaçamento temporal. Verificou-se que a sua concretização está dependente do tipo de equipamento de calibração e da natureza quer dos elementos sensíveis às variações de temperatura, que constituem o termopar a calibrar, quer dos materiais que os protegem mecanicamente. Consequentemente, impõe-se a necessidade de algum conhecimento prévio das características estáticas e dinâmicas dos dispositivos a calibrar.

Para a calibração em valores contínuos utilizou-se o modelo dos mínimos quadrados ponderados. É utilizado o método de Gauss-Newton para a determinação dos parâmetros do polinómio de interpolação, de forma a considerar as não linearidades introduzidas pela incerteza presente nas duas variáveis, medidas da grandeza de referência e da grandeza a calibrar. Este método permite validar o modelo mais expedito e numericamente menos pesado que toma em consideração apenas uma incerteza equivalente no valor medido da grandeza a calibrar.

# ON PM TUBULAR LINEAR SYCCHRONOUS MOTOR MODELLING

**Luís, Ricardo; Quadrado, José Carlos**

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Lisboa, Portugal

In this paper a new approach is made on PM tubular linear synchronous motor (PM-TLSM) modelling, considering a non linear model. This model allows the incorporation of PM elements characteristics. The straight forward approach induces robust simulation results for tubular linear machines, without resorting to complex variable transformations.

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*WSEAS TRANSACTIONS  
on CIRCUITS and  
SYSTEMS, Issue 9,  
Volume 3  
ISSN: 1109-2734,  
November 2004.*

# MODELLING A 6 DOF ELECTROMECHANICAL PLATFORM

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Lisboa, Portugal

In this paper the kinematics and dynamic model of a six-degree-of-freedom, 6-DOF, Platform using electromechanical actuators is presented. A 6 DOF platform in development displays the advantages of using electromechanical actuators. The kinematics and dynamic of an universal, prismatic and spherical joints set, known as UPS set is modelled. Kinematics and dynamics of the platform are also included. Several details of this platform are depicted.

**Publicado em:**

*WSEAS TRANSACTIONS  
on SYSTEM, Issue 10,  
Volume 3  
ISSN: 1109-2777,  
December 2004.*

# UNIVERSAL MOTOR NN MODELLING

**Quadrado, José Carlos**

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The paper presents a hybrid modelling of electrical motors. To improve the performance, the analytical model is combined with Adaptive-Network-based Fuzzy Inference System (ANFIS) to compensate the modelling error. The architecture and hybrid learning procedure is presented. The method is applied to universal motors. In the first step, parameters of analytical model are identified by simple least-square method. Then, the modelling error is compensated by hybrid learning procedure, preserving the meaning of the physical parameters. The reliability of the obtained model is increased.

**Publicado em:**  
*WSEAS TRANSACTIONS  
on CIRCUITS and  
SYSTEMS, Issue 10,  
Volume 3  
ISSN: 1109-2734,  
December 2004.*

# USAGE OF AN ASYMMETRICAL ROTATING INDUCTION MOTOR TO OBTAIN A LIM DYNAMIC MODEL

**Quadrado, José Carlos**

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The aim of this paper is to present a new model for the linear induction motor (LIM), which is based on its equivalence with the asymmetrical rotary induction motor. The model uses the theory of positive, negative and zero sequence of symmetrical and asymmetrical components. Experimental and simulation procedures with a LIM prototype allowed the theoretical and experimental validation for this model.

**Publicado em:**

*WSEAS  
TRANSACTIONS on  
CIRCUITS and  
SYSTEMS, Issue 4,  
Volume 3  
ISSN: 1109-2734,  
June 2004.*

# FONTES DE ALTA TENSÃO PULSADA PARA IMPLANTAÇÃO IÓNICA DE IMERSÃO EM PLÁSMAS

**Redondo, Luís Manuel dos Santos**

**Doutoramento em:** Engenharia Electrotécnica e de Computadores.

**Grau Concedido por:** IST – Universidade Técnica de Lisboa.

**Orientadores:** Doutor José Fernando Alves Silva (orientador científico e Professor Associado do IST), Doutor Elmano da Fonseca Margato (co-orientador científico e Professor Coordenador do ISEL), Doutor José Carvalho Soares (co-orientador científico e Professor Catedrático da FC da UL).

**Provas Concluídas em:** 24 de Julho de 2004.

Propõem-se novas topologias de conversores electrónicos de potência e arquitecturas de transformadores para obter impulsos quase rectangulares de tensão elevada (vários kV). Tal permite definir metodologias para obter Fontes de Alta Tensão Pulsada (FATP) para aplicação em Implantação Iónica de Imersão em Plasma (IIIP), utilizando dispositivos semicondutores de potência (DSP) de baixa tensão (<1 kV), sem usar associações em série. Referem-se as potencialidades da associação de DSP em circuitos do tipo “gerador de Marx”. Desenvolve-se uma FATP elementar, baseada num conversor modificado, alimentado em corrente contínua, que aproveita a operação com baixo factor de ciclo e a reduzida tensão da malha de desmagnetização do transformador elevador, para reduzir a tensão máxima nos DSP. Partindo desta FATP elementar, uma concepção modular permite construir FATP capazes de gerar os impulsos adequados aos processos de IIIP. Concebem-se, analisam-se e projectam-se transformadores para impulsos de tensão elevada, que usam enrolamentos auxiliares para compensar fenómenos de dispersão magnética. Nos transformadores construídos, os tempos de subida do impulso são reduzidos entre 20 % e 98 %, em relação ao transformador sem enrolamentos auxiliares.

O protótipo laboratorial modular construído tem rendimento energético de aproximadamente 80 %, sendo capaz de fornecer, a cargas resistivas absorvendo 1 A, impulsos de tensão de amplitude -15 kV, largura 5  $\mu$ s, frequência 10 kHz, com tempos de subida inferiores a 1  $\mu$ s.

# UM MODELO INTEGRADO DE SISTEMAS EÓLICOS EQUIPADOS COM MÁQUINAS SÍNCRONAS DE VELOCIDADE VARIÁVEL

## Conceição, Mário Rui Melício da

**Mestrado em:** Engenharia Electrotécnica e de Computadores.

**Grau Concedido por:** IST – Universidade Técnica de Lisboa.

**Orientadores:** Doutor Rui Manuel Gameiro de Castro (orientador científico e Professor Auxiliar do IST) e Doutor Victor Manuel Fernandes Mendes (co-orientador científico e Professor Coordenador do ISEL).

**Provas Concluídas em:** 08 de Outubro de 2004.

Nos últimos anos tem aumentado a importância do uso de energias não poluentes e renováveis que não contribuem para o efeito de estufa, contribuindo para a redução dos problemas ambientais associados à utilização das fontes de energia baseadas em combustíveis fósseis. A incorporação de fontes de energia renováveis, contribuindo para diminuir o recurso às centrais térmicas no sistema produtor eléctrico, é uma medida importante na prossecução do objectivo de reduzir as emissões poluentes para a atmosfera, cumprindo o Protocolo de Quioto.

Os dados disponíveis indicam que em Portugal, os sistemas eólicos equipados com interfaces de electrónica de potência e geradores síncronos de velocidade variável representam uma das soluções mais utilizadas para os sistemas instalados e em fase de construção até 2003, mas para 2004 espera-se que a máquina de indução de rotor bobinado venha a conquistar vantagem.

Os sistemas eólicos equipados com turbinas eólicas directamente ligadas a máquinas síncronas de velocidade variável e interfaces de electrónica de potência constituem o âmbito da contribuição desta tese. Esta dissertação aborda mais particularmente dois estudos: o modelo dinâmico de uma turbina eólica de três pás posicionadas de forma equilibrada com eixo horizontal, controlando o ângulo do passo da pá; os sistemas eólicos equipados com turbinas eólicas directamente ligadas a máquinas síncronas de velocidade variável, usando interfaces de electrónica de potência, que é a configuração de conversão de energia eléctrica mais usada em aproveitamentos de energia eólica.





06

# FÍSICA

Anuário Científico 2004

ISEL



# BOUNDS ON GAMMA FROM CP VIOLATION MEASUREMENT IN $B \rightarrow \pi^+ \pi^-$ AND $B \rightarrow \pi^+ \pi^- K_S$

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We study the determination of  $\gamma$  from CP-violating observables in  $B \rightarrow \pi^+ \pi^-$  and  $B \rightarrow \pi^+ \pi^- K_S$ . This determination requires theoretical input to one combination of hadronic parameters. We show that a mild assumption about this quantity may allow bounds to be placed on  $\gamma$ , but we stress the pernicious effects that an eightfold discrete ambiguity has on such an analysis. The bounds are discussed as a function of the direct (C) and interference (S) CP-violating observables obtained from time-dependent  $B \rightarrow \pi^+ \pi^-$  decays, and their behaviour in the presence of new physics effects in B-Bbar mixing is studied.

**Publicado em:**

*Physical Review D*, 70, 096007, 2004.

# LASER-ASSISTED DEPOSITION OF THIN FILMS FROM PHOTOEXCITED VAPOUR PHASES

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**Publicado em:**  
*Applied Physics A*, 79,  
489 – 497, 2004  
(invited paper).

Laser-assisted chemical vapour deposition (LCVD) has been extensively studied in the last two decades. A vast range of applications encompass various areas such as microelectronics, micromechanics, microelectromechanics and integrated optics, and a variety of metals, semiconductors and insulators have been grown by LCVD. In this article, we review briefly the LCVD process and present two case studies of thin film deposition related to laser thermal excitation (e.g. boron carbide) and non-thermal excitation (e.g. CrO<sub>2</sub>) of the gas phase.

# KRF PULSED LASER DEPOSITION OF CHROMIUM OXIDE THIN FILMS FROM $\text{Cr}_8\text{O}_{21}$ TARGETS

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In this work, we describe our efforts to grow chromium oxide thin films by PLD from  $\text{Cr}_8\text{O}_{21}$  targets, using a KrF excimer laser. The as-deposited films were investigated by X-ray diffraction and Rutherford backscattering spectrometry. Structural and chemical composition studies showed that the films consist of a mixture of amorphous chromium oxides exhibiting different stoichiometries depending on the processing parameters, where nanocrystals of mainly  $\text{Cr}_2\text{O}_3$  are dispersed. The analyses do not exclude the possibility of co-deposition of  $\text{Cr}_2\text{O}_3$  and a low fraction of  $\text{CrO}_2$ .

**Publicado em:**

*Applied Physics A*, 79,  
1409 – 1411, 2004.

# KrF LASER CVD OF CHROMIUM OXIDE BY PHOTODISSOCIATION OF $\text{Cr}(\text{CO})_6$

**Sousa, P.M.<sup>1</sup>; Silvestre, A.J.<sup>2</sup>; Popovici, N.<sup>1</sup>;  
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This work reports on the synthesis of chromium oxide thin films prepared by photodissociation of  $\text{Cr}(\text{CO})_6$  in an oxidizing atmosphere, using a pulsed UV laser (KrF,  $\lambda = 248 \text{ nm}$ ). The experimental conditions which should enable the synthesis of  $\text{CrO}_2$  are discussed and results on the deposition of  $\text{Cr}_x\text{O}_y$  films on  $\text{Al}_2\text{O}_3$  (0001) substrates are presented.

**Publicado em:**

*Materials Science  
Forum, 455, 20 – 24,  
2004.*

# SOME ASPECTS OF RHEO-NMR BEHAVIOUR OF THE LYOTROPIC LIQUID CRYSTAL POLY( $\gamma$ -BENZYL-L-GLUTAMATE) IN *m*-CRESOL

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We use  $^2\text{H}$  NMR spectroscopy to study the director orientation in two nematic solutions of poly( $\gamma$ -benzyl-L-glutamate) (PBLG) in *m*-cresol during simple shear-flow and after its sudden cessation. In the range of applied shear rates ( $\dot{\gamma} = 5 \dots 150 \text{ s}^{-1}$ ), a steady state NMR line shape is reached after a deformation of a few hundred units. Two different line shapes occur, that can be related to distinct shear responses in mechanical rheology: the tumbling/wagging and the flow-aligning regimes. The relaxation after cessation of the shear is similar for both cases, and essentially follows the “inhomogeneous reorientation” regime known from sudden-rotation NMR experiments. A fit of the relaxation curves indicates that the tumbling parameter  $\lambda$  is (slightly) less than one, as expected for a tumbling system.

**Publicado em:**  
*Molecular Crystal and  
Liquid Crystals*, 420,  
35, 2004.

# DIFFUSION-LIMITED DEPOSITION OF DIPOLAR PARTICLES

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**Publicado em:**  
*Physical Review E, Vol.*  
*69, 061406, 2004.*

Deposits of dipolar particles are investigated by means of extensive Monte Carlo simulations. We found that the effect of the interactions is described by an initial, nonuniversal, scaling regime characterized by orientationally ordered deposits. In the dipolar regime, the order and geometry of the clusters depend on the strength of the interactions and the magnetic properties are tunable by controlling the growth conditions. At later stages, the growth is dominated by thermal effects and the diffusion-limited universal regime obtains, at finite temperatures. At low temperatures the crossover size increases exponentially as  $T$  decreases and at  $T = 0$  only the dipolar regime is observed.

# INTERACTION OF COLLOIDS WITH A NEMATIC-ISOTROPIC INTERFACE

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The Landau-de Gennes free energy is used to calculate the interaction between long cylindrical colloids and the nematic-isotropic (NI) interface. This interaction has two contributions: one is specific of liquid crystals and results from the deformation of the director field close to the particles or to the interface, while the other is generic and results from wetting and surface tension effects. Deep in the nematic phase the director field of long cylindrical colloids, with strong homeotropic anchoring, exhibits two half-integer defect lines. As the colloid moves towards the interface, the director configuration changes through a series of discontinuous transitions, where one or two of the defects are annihilated. In addition, the NI interface bends towards the colloid in order to minimize the elastic free energy in the nematic. In the isotropic phase, the colloid is surrounded by a thin nematic layer that reduces the surface free energy under favorable wetting conditions. The interaction has a well-defined minimum near the interface. In this region the director and interfacial structures are complex and cannot be described analytically. Using the numerical results for the Landau-de Gennes free energy in the harmonic region, we obtained simple scaling laws for the (linear) force on the colloid.

**Publicado em:**

*Physical Review E, Vol. 69, 021706, 2004.*

# COLLOIDAL DISCS IN NEMATIC LIQUID CRYSTALS

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We use adaptive finite elements methods to investigate a variety of structures in inverted nematic emulsions numerically. In particular, we study dipolar and quadrupolar interactions between colloidal discs in two-dimensional nematics. The behaviour of colloidal particles near a substrate and at a nematic-isotropic interface are also considered.

**Publicado em:**

*J. Phys.: Condens.  
Matter, Vol. 16, S1921,  
2004.*

# KEY-LOCK MECHANISM IN NEMATIC COLLOIDAL DISPERSIONS

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We consider the interaction between two-dimensional nematic colloids and planar or sculpted walls. The elastic interaction between colloidal disks and flat walls, with homeotropic boundary conditions, is always repulsive. These repulsions may be turned into strong attractions at structured or sculpted walls, with cavities that match closely the shape and size of the colloids. This key-lock mechanism is analyzed in detail for colloidal disks and spherocylindrical cavities of various length to depth ratios, by minimizing the Landau-de Gennes free energy functional of the nematic orientational order parameter. We find that the attractions occur only for walls with cavities within a small range of the colloidal size and a narrow range of orientations with respect to the cavity's symmetry axis.

**Publicado em:**

*Physical Review E, Vol.  
69, 061402, 2004.*

# CAPILLARY BRIDGING AND LONG-RANGE ATTRACTIVE FORCES IN A MEAN-FIELD APPROACH

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When a mixture is confined, one of the phases can condense out. This condensate, which is otherwise metastable in the bulk, is stabilized by the presence of surfaces. In a sphere-plane geometry, routinely used in atomic force microscope and surface force apparatus, it, can form a bridge connecting the surfaces. The pressure drop in the bridge gives rise to additional long-range attractive forces between them. By minimizing the free energy of a binary mixture we obtain the force-distance curves as well as the structural phase diagram of the configuration with the bridge. Numerical results predict a discontinuous transition between the states with and without the bridge and linear force-distance curves with hysteresis. We also show that similar phenomenon can be observed in a number of different systems, e.g., liquid crystals and polymer mixtures.

**Publicado em:**

*J. Chem. Phys.*, Vol.  
121, 4414, 2004.

# PORTUGUESE SEISMIC NETWORKS

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- 3** Instituto de Meteorologia, Lisboa

Portugal is an area of moderate to high seismic activity. In the past, the Portuguese territory has been affected by large earthquakes, like the 1755 1st of November earthquake which destroyed Lisbon and caused more than 30 000 casualties. More recently, during the last century, the Azores islands have also suffered significant human and economic losses.

The very first installation of seismographic stations in Portugal occurred in the dawn of the former century. In 1902, two Milne pendulae have been deployed at the Azores islands, one in Ponta Delgada (São Miguel) and the other in Horta (Faial). Since then, and for almost eight decades, the development of seismology in Portugal always followed large earthquakes. In the aftermath of these earthquakes (mainly 1909, April 23rd; 1969, February 28th and 1980, January 1st) a few initiatives have been taken to expand the national seismic network. In the last two decades, several programmes have been started by different institutions to improve the seismic surveillance of the Portuguese territory.

The ex Instituto Nacional de Meteorologia e Geofísica, now Instituto de Meteorologia (IM), has been for a long time the main responsible for the portuguese seismic network. Nowadays, several groups are running a pool of seismic stations. The Instituto de Meteorologia continues to be the portuguese coordinator of national network, which is mainly devoted to the seismic surveillance of the portuguese economic zone. Other groups, connected to some Portuguese Universities, run seismic stations for research studies.

**Publicado em:**  
*Orfeus Newsletters*  
*Electronic Newsletter,*  
*6, nº 1, 2004*

# PHENOMENOLOGICAL ASPECTS OF CP VIOLATION

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We present a pedagogical review of the phenomenology of CP violation, with emphasis on B decays.

Main topics include the phenomenology of neutral meson systems, CP violation in the Standard Model of electroweak interactions, and B decays.

We stress the importance of the reciprocal basis, sign conventions, rephasing invariance, general definitions of the CP transformation and the spurious phases they bring about, CP violation as originating from the clash of two contributions, the rho-eta plane, the four phases of a generalized CKM matrix, and the impact of discrete ambiguities.

Specific B decays are included in order to illustrate some general techniques used in extracting information from B physics experiments.

We include a series of simple exercises. The style is informal.

**Publicado em:**

*e-Print Archive: hep-ph/0410351; invited talk at Central European School in Particle Physics, Prague, Czech Republic, 14-24 September, 2004.*

# CrO<sub>2</sub>/Cr<sub>2</sub>O<sub>3</sub> BIPHASIC FILMS OBTAINED FROM KRF LASER PHOTODISSOCIATION OF Cr(CO)<sub>6</sub>

Silvestre, A.J.<sup>1</sup>; Sousa, P.M.<sup>2</sup>; Popovici, N.<sup>2</sup>;  
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In recent years, there has been much interest in magnetoresistive oxide films due to their usage in magneto-electronic devices. Among them, biphasic CrO<sub>2</sub>/Cr<sub>2</sub>O<sub>3</sub> films show remarkable magnetoresistance due to intergrain tunneling between high spin polarized crystals. However, their synthesis at low temperature has been a difficult task due to the metastability of CrO<sub>2</sub>.

This work reports on the synthesis of chromium oxide films by KrF laser-assisted CVD. Films were grown onto Al<sub>2</sub>O<sub>3</sub> (1000) substrates at room temperature by photodissociation of Cr(CO)<sub>6</sub> in dynamic atmospheres containing O<sub>2</sub> and Ar. The deposited material was analysed by X-ray diffraction, micro-Raman spectroscopy and scanning electron microscopy. The films display a behaviour consistent with a two-phase system holding both Cr<sub>2</sub>O<sub>3</sub> and CrO<sub>2</sub> oxides. They present a microstructure consisting mainly of granular and rod-shaped particles ranging from 300 nm to 3 μm in size. A study of the processing parameters has shown that partial pressure ratio  $p_{\text{Cr(CO)}_6}/p_{\text{O}_2}$  and laser fluence are the prominent parameters that have to be carefully controlled in order to increase the content of CrO<sub>2</sub> in the deposited films.

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*Livro de resumos da  
"4th International  
Conference on  
Photoexcited  
Processes &  
Applications,  
ICPEPA'04, Lecce,  
Italy, 2004.*

# TiO<sub>2</sub> AND Co-DOPED TiO<sub>2</sub> THIN FILMS GROWN BY PULSED LASER DEPOSITION

Popovici, N.<sup>1</sup>; Sousa, P.M.<sup>1</sup>; Silva, R.C.<sup>2</sup>;  
Paramês, M.L.<sup>1</sup>; Silvestre, A.J.<sup>3</sup>; Axelsson, A.K.<sup>4</sup>;  
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Titanium dioxide is one of the most extensively studied transition metal oxides because of its remarkable optical and electronic properties. TiO<sub>2</sub> anatase polymorph is a wide band-gap semiconductor with excellent optical transmission in the visible and near-infrared regions, high refractive index and dielectric constant. Recently, Co-doped (anatase) TiO<sub>2</sub> was found to exhibit ferromagnetic properties. In this work, we report on the growth of undoped and Co-doped anatase TiO<sub>2</sub> thin films on heated Si(100) substrates by pulsed laser deposition (PLD) using a KrF Laser. Both TiO<sub>2</sub> and Co-TiO<sub>2</sub> rutile sintered pellets were used as targets.

The as-deposited films were characterised by X-ray Diffraction (XRD), Energy Dispersive Spectrometry (EDS), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), and Ellipsometry. The films deposited from undoped targets consist of polycrystalline anatase with a refractive index of 2.25. Films obtained from the Co-doped targets present the anatase phase embedded in an amorphous matrix, an atomic content of Co that varies with target composition, and a refractive index of about 2.28.

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*Livro de resumos da  
"4th International  
Conference on  
Photoexcited  
Processes &  
Applications,  
ICPEPA'04, Lecce,  
Italy, 2004.*

# MORPHOLOGICAL AND STRUCTURAL CHARACTERIZATION OF $\text{CrO}_2/\text{Cr}_2\text{O}_3$ FILMS GROWN BY LASER-CVD

Sousa, P.M.<sup>1</sup>; Silvestre, A.J.<sup>2</sup>; Popovici, N.<sup>1</sup>; Conde, O.<sup>1</sup>

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In recent years, there has been much interest in magnetoresistive oxide films due to their usage in magneto-electronic devices. Among them,  $\text{CrO}_2/\text{Cr}_2\text{O}_3$  composites show remarkable magnetoresistance. However, their synthesis at low temperature has been a difficult task due to the metastability of  $\text{CrO}_2$ . In this work we report on the synthesis of chromium oxide films by KrF laser-assisted CVD. Films were deposited onto sapphire substrates at room temperature by photodissociation of  $\text{Cr}(\text{CO})_6$  in dynamic atmospheres containing oxygen and argon. The deposited material was analysed by X-ray diffraction, micro-Raman spectroscopy and scanning electron microscopy. The as-deposited films were characterised by X-ray Diffraction (XRD), Energy Dispersive Spectrometry (EDS), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM) and Ellipsometry. The films deposited from undoped targets consist of polycrystalline anatase with a refractive index of 2.25. Films obtained from the Co-doped targets present the anatase phase embedded in an amorphous matrix, an atomic content of Co around 7 % and a refractive index about 2.28.

**Publicado em:**

*Livro de resumos da conferência "E-MRS'04 Spring Meeting", Symp. N, Strasbourg, France, 2004.*

# PULSED LASER DEPOSITION OF TiO<sub>2</sub> AND Co-DOPED TiO<sub>2</sub> THIN FILMS

Popovici, N.<sup>1</sup>; Sousa, P.M.<sup>1</sup>; Paramês, M.L.<sup>1</sup>;  
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Titanium dioxide is one of the most extensively studied transition metal oxides because of its remarkable optical and electronic properties. TiO<sub>2</sub> anatase polymorph is a wide band-gap semiconductor with excellent optical transmission in the visible and near-infrared regions, high refractive index and dielectric constant. Recently, Co-doped (anatase) TiO<sub>2</sub> was found to exhibit ferromagnetic properties. In this paper, we report on the growth of undoped and Co-doped anatase TiO<sub>2</sub> thin films onto heated Si(100) substrates by pulsed laser deposition (PLD), using a KrF laser. Pure TiO<sub>2</sub> and 8 wt.% Co-TiO<sub>2</sub> rutile targets were used. The as-deposited films were characterised by X-ray Diffraction (XRD), Energy Dispersive Spectrometry (EDS), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM) and Ellipsometry. The films deposited from undoped targets consist of polycrystalline anatase with a refractive index of 2.25. Films obtained from the Co-doped targets present the anatase phase embedded in an amorphous matrix, an atomic content of Co around 7 % and a refractive index about 2.28.

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conferência "E-MRS'04  
Spring Meeting",  
Symp. N, Strasbourg,  
France, 2004.*

# INFLUENCE OF LCP CONTENT AND COMPATIBILIZER STRUCTURE ON THE MORPHOLOGICAL, RHEOLOGICAL AND MECHANICAL PROPERTIES OF COMPATIBILIZED PP/LCP

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The use of thermoplastic/liquid crystalline polymer blends is recognized as a good strategy to reduce the viscosity and to improve the mechanical properties relatively to those of pure thermoplastic. The addition of compatibilizers to LCP/TP blends is generally needed to improve the adhesion between the two components, guarantying the reduction of fibril's pullout and thus, the mechanical improvement relatively to that of non-compatibilized blends. In this work, the study of morphological, rheological and mechanical properties was performed for LCP/TP blends, considering the influence of the use of different compatibilizers and different LCP contents.

**Publicado em:**

*Proceedings of XIVth International Congress on Rheology, Edited by The Korean Society of Rheology, Seoul, Korea, August 2004*

# DIFFUSION LIMITED DEPOSITION OF DIPOLAR PARTICLES

**Santos, F. de los<sup>1</sup>; Tavares, J.M.<sup>2,3</sup>;  
Tasinkevych, M.<sup>4</sup>; Gama, M.M. Telo da<sup>2,5</sup>**

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Congresso "SIMU  
2004 – Bridging the  
scales", p. 38, Agosto  
de 2004.*

Deposition of dipolar particles under diffusion-limited conditions are investigated by means of extensive Monte Carlo simulations. It is found that the effect of the interactions on the size and shape of the deposits may be described by an initial, non-universal, scaling regime characterized by the formation of orientationally ordered deposits. In the dipolar regime, the orientational order, the shape and the fractal dimension of the clusters depend on the strength of the dipolar interactions and thus the magnetic properties of the deposits may be tuned by controlling the growth conditions, such as temperature. At a later stage, the growth is dominated by thermal effects and the universal scaling regime of diffusion-limited deposition obtains, at finite temperatures. At low temperatures the crossover increases exponentially as  $T$  decreases and only the dipolar regime is observed at  $T=0$ .

# THE NATURE OF THE PHASE TRANSITION IN DIPOLAR FLUIDS

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Monte Carlo computer simulations of a quasi two dimensional dipolar fluid at low and intermediate densities indicate that the structure of the fluid is well described by an ideal mixture of self-assembling clusters. A detailed analysis of the topology of the clusters, of their internal energy and of their size (mass) distributions further suggest that the system undergoes a phase transition from a dilute phase characterized by a number of disconnected clusters to a condensed phase characterized by a network or spanning (macroscopic) cluster that includes most of the particles in the system.

**Publicado em:**

*Livro de resumos de  
"Conference on  
Computational Physics  
- CCP2004", p. 181,  
Setembro de 2004.*

# THE KEY-LOCK MECHANISM IN NEMATIC COLLOIDAL DISPERSIONS

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**Publicado em:**  
*Abstract book of  
Statphys 22 (2004).*

We consider the effect of planar or sculpted walls in two-dimensional colloidal dispersions in nematics. The behavior of colloidal particles in a nematic matrix depends upon (i) the elastic constants of the nematic, (ii) the size of the particle, and (iii) the boundary conditions at the particle and at the container. The elastic interaction between a colloidal disc and a flat wall, with homeotropic boundary conditions, is always repulsive. The repulsions are turned into strong attractions at structured or sculpted walls, with cavities that match closely the shape and size of the colloids. This key-lock mechanism is analyzed in detail for colloidal disks and spherocylindrical cavities of various length to depth ratios, by minimizing the Landau-de Gennes free energy functional of the nematic orientational order parameter. We find that the attractions occur only for walls with cavities within a small range of the colloidal size and for a narrow range of orientations around the symmetry axis of the cavity.

# JOINT INVERSION OF RECEIVER FUNCTIONS AND MAGNETOTELLURIC-PRELIMINARY RESULTS

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Receiver function analysis is now widely used to infer 1-D shear-wave velocity distributions with depth. This method, mainly sensitive to shear velocity contrasts and vertical travel times, suffers from a trade-off between the velocity contrast and the depth where it occurs. On the other hand, magnetotelluric is widely used to infer electrical conductivity distribution with depth.

Receiver functions (RF) and magnetotelluric (MT) can be simultaneously employed to retrieve shear wave velocity and electrical conductivity distributions with depth in the lithosphere assuming a common layered earth. It is expected that the combination of the two geophysical measurements yields a better-constrained (velocity and conductivity) model. The preliminary results (based on synthetic data) obtained with a program developed to perform the joint inversion of RF and MT data are presented and discussed in this communication.

**Publicado em:**

*Livro de resumos da  
4.<sup>a</sup> Assembleia Luso-  
Espanhola de  
Geodesia e Geofísica,  
Figueira da Foz, 3-7  
Fevereiro, 2004.*

# AZORES HOTSPOT AS SEEN BY TOMOGRAPHIC MODELS

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**Publicado em:**  
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 4ª Assembleia Luso-  
 Espanhola de  
 Geodesia e Geofísica,  
 Figueira da Foz, 3-7  
 Fevereiro, 2004.*

The Azores exhibits a complex tectonic setting due to the existence of the Azores hotspot and to the eventual hotspot-ridge interaction. The hotspot origin at depth as a plume and its lateral extent are controversial subjects. High-resolution tomographic models can provide an important hint to evaluate the depth and lateral extent of mantle plumes. We investigate the Azores deep seismic structure as seen on recent global and regional studies. The mapping of S-wave negative velocity anomalies in the different models reveals that the anomaly right beneath the Azores seems to be confined in the upper 200km. Considering the time evolution of a plume, this low velocity anomaly might be the signature of a present-day dying plume, that created the Azores plateau 20Ma ago. In the model from Silveira and Stutzmann (2002), the negative velocity anomaly beneath the Azores archipelago seems to be connected to a deep anomaly further at the South. This deep anomaly (28°N/26°W, 200-400km) is in the middle of the bunch of Azores, Great Meteor, Madeira and Canary hotspots, and might be related to a plume originating either in the transition zone or in the lower mantle. This single deep plume is located too far from the Azores archipelago for being responsible of the Azores plateau formation. But, due to the lithosphere geometry, this single plume might feed at present day Azores, Great Meteor, Madeira, Canaries and Cape Verde hotspots and therefore be at the origin of the present day volcanism. The diverging azimuthal anisotropy around this point below lithosphere is confirming a unique origin of these hotspots.

# 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 the central and western Iberia. A better characterization of mantle anisotropy beneath is important, not only at this part of the Iberian Peninsula, but 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 Península, 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 zones have often, but not universally, indicated a fast axis parallel to the orogen, which is consistent with collisional shortening of the mantle root (Silver, 1996). Our preliminary SKS measurements beneath MTE seem to confirm this result.

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# AZORES CRUSTAL STRUCTURE FROM RECEIVER FUNCTIONS

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The Azores archipelago occupies a lateral branch of the Mid-Atlantic ridge near the triple junction of 3 large tectonic plates, the North American, the Eurasian and the African plates. The tectonic setting is even more complex due to the existence of the Azores hotspot. Its origin is still controversial. Besides, due to this complex tectonic environment, the Azores lithosphere, and especially the crustal part, exhibits important deep and lateral variations in both structure and composition. We intend to characterize the structure just beneath each VBB seismic station, deployed in the framework of the Memorandum of Understanding COSEA, by the receiver function analysis.

# THERMOCHEMICAL INSTABILITIES IN THE INDO-ATLANTIC MANTLE OVER THE LAST 260 MYR

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Using recent fluid mechanics results as a framework, we reinterpret the images of the Indo-Atlantic mantle obtained from global and regional tomography studies together with geochemical, geological and paleomagnetic observations to unravel the pattern of convection in the Indo-Atlantic "box" and its temporal evolution over the last 260 Myr. Seismic tomography sections at different depths show that the Earth's mantle seems to be divided in two "boxes" by the subducted plates, the Pacific and the Indo-Atlantic boxes. The latter presently contains a) a broad slow seismic anomaly at the CMB, which divides into several branches higher in the lower mantle, b) one "superswell" centered on the western edge of South Africa, c) at least 5 "primary hotspots" with long tracks related to traps, and d) numerous smaller hotspots. Moreover, in the last 260 Myr, this mantle box has undergone 10 traps events, 7 of them related to continental break up. Several of these past events are spatially correlated with present-day seismic anomalies and/or upwellings, suggesting episodicity. Laboratory experiments led us to propose that superswells, long-lived hot spot tracks and traps may represent three stages of the same phenomenon: the episodic destabilization of a hot thermal boundary layer lying close to the bottom of the mantle and containing chemical heterogeneities. This could produce thermochemical plumes, either with large heads (traps) and thin tails (tracks) if less viscous than the ambient mantle, or fingerlike domes if more viscous than the ambient mantle. The recurrence of this phenomenon in the mantle would be 100-200 Myr with a wavelength of 2000-4000 km at the CMB, in agreement with observations.

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# REVISÃO DA SEQUÊNCIA SÍSMICA DO FAIAL DE 9-7-1998

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 Nacional de  
 Sismologia e  
 Engenharia Sísmica,  
 Guimarães, Portugal,  
 Abril de 2004.*

Em Julho de 1998 foi instalada uma rede sísmica digital móvel nas ilhas Faial, Pico e S. Jorge, para a monitorização da sequência sísmica desencadeada pelo sismo do Faial de 9 de Julho. A resolução dos problemas instrumentais e a revisão de toda a informação disponível, permitiu incrementar significativamente a base de dados disponível para análise, o que motivou a reanálise de resultados anteriormente obtidos. Seguindo-se a metodologia anteriormente utilizada, foi seleccionado o conjunto de dados para os quais se dispunha da melhor cobertura azimutal, após o que se efectuou a realocização dos eventos usando a metodologia de Kissling et. al (1994), que permite a inversão simultânea do modelo 1-D, determinação das correcções de estação e determinação hipocentral. Em resultado, a distribuição espacial dos eventos ficou mais organizada, obtendo-se um menor RMS global e definindo-se várias áreas de geração sísmica; estas áreas foram refinadas recorrendo a técnicas de taxonomia aplicadas à forma da onda sísmica. Para cada uma das áreas em causa foi calculado o mecanismo composto por inversão das polaridades da onda P, e para os eventos melhor constrangidos ( $n^o$  de polaridades  $\geq 11$ ) foram calculados os mecanismos focais singulares. Os resultados obtidos sugerem que a actividade sísmica envolveu outras falhas próximas para além da que originou o sismo principal, o que está de acordo com outras observações tectónicas e geoquímicas efectuadas.

# CONTROLO DE RUÍDO NA INDÚSTRIA MINEIRA

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A entrada em vigor, em 14 de Maio de 2001, do Regime Legal sobre a Poluição Sonora, (anexo ao Decreto-Lei nº 292/2000 de 14 de Novembro), determinou que as actividades ruidosas já existentes disporiam de 1 ano a partir dessa data para implementar as medidas necessárias ao cumprimento dos critérios estabelecidos naquele documento legal. A Indústria Portuguesa teve, então, de encetar esforços no sentido de rapidamente se adaptar àquele regime jurídico. Neste artigo, os autores apresentam, como caso particular, as acções de engenharia acústica desenvolvidas para uma das mais importantes empresas portuguesas na área da indústria mineira: SOMINCOR - Sociedade Mineira de Neves Corvo.

No sentido de controlar as respectivas emissões de ruído para a comunidade envolvente, a SOMINCOR promoveu não só o levantamento de ruído na sua envolvente exterior, como implementou, na suas naves e/ou equipamentos, medidas técnicas de controlo de ruído.

É apresentada a metodologia seguida pelos autores do trabalho com vista à redução dos níveis de ruído gerados na exploração mineira e que consistiu, nomeadamente, na modelação e simulação da emissão das fontes sonoras predominantes e na elaboração dos correspondentes mapas de ruído para diferentes cenários, quer para o interior da unidade quer para a área envolvente exterior. A informação das cartas de ruído foi complementada com um extenso programa de medições acústicas no interior e no exterior da instalação.

Com base na informação constante das cartas de ruído elaboradas, foram dimensionadas e especificadas as adequadas medidas de redução de ruído. Os benefícios foram avaliados através dos métodos previsionais.

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Congresso  
Internacional  
ACÚSTICA 2004,  
Guimarães, Portugal,  
Setembro de 2004.*

# PARQUES EÓLICOS - ESTUDO DOS IMPACTES NO AMBIENTE SONORO. I - INFLUÊNCIA NO RUÍDO LOCAL

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Congresso  
Internacional  
ACÚSTICA 2004,  
Guimarães, Portugal,  
Setembro de 2004.*

A crescente procura pela comunidade internacional de novas formas de energia, nomeadamente de energia limpa e renovável, tem determinado a proliferação de Parques Eólicos. Também em Portugal, a opção pela Energia Eólica tem vindo a acompanhar esta tendência, tanto mais que as condições naturais existentes no nosso País assim o favorecem. De qualquer forma, a implantação de um Parque Eólico origina uma potencial alteração do ambiente sonoro local, pelo que a sua influência deve ser convenientemente estudada e, quando necessário, controlada e/ou minimizada na proximidade de comunidades ou núcleos habitacionais. Os autores deste artigo, cuja experiência em Estudos Acústicos de Parques Eólicos e de aerogeradores é significativa e consistente, apresentam as metodologias seguidas na análise dos efeitos observados no ruído ambiente da zona de implantação de um Parque Eólico, bem como a especificação otimizada das características dos aerogeradores, em 2 artigos subordinados ao tema: *Parques Eólicos - Estudo dos Impactes no Ambiente Sonoro: I) Influência no Ruído Local; II) Configuração Otimizada de Potências Sonoras*. Neste primeiro artigo (*I - Influência no Ruído Local*), são evidenciadas as influências do ruído gerado pelos aerogeradores de um Parque Eólico no ambiente sonoro local. É referido, de forma clara, o cuidado e a atenção a ter na correspondente análise de impactes, nomeadamente no que respeita à adequada caracterização da Situação de Referência. Factores, como, por exemplo, a velocidade do vento, são determinantes para a correcta avaliação dos impactes no ambiente sonoro. São apresentados e descritos casos exemplares. É, também, exemplificado, neste artigo, a caracterização de uma Situação de Referência, bem como os correspondentes acréscimos de ruído que se prevêm durante a plena exploração de um Parque Eólico. Em artigo complementar (*II - Configuração Otimizada de Potências Sonoras*), é mostrado que através da optimização da Potência Sonora dos aerogeradores é possível minimizar os efeitos do ruído produzido por um Parque Eólico.

# PARQUES EÓLICOS - ESTUDO DOS IMPACTES NO AMBIENTE SONORO. II - CONFIGURAÇÃO OPTIMIZADA DE POTÊNCIAS SONORAS

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A implantação de um Parque Eólico pode originar a alteração do ambiente sonoro local, pelo que a sua influência deve ser estudada e, quando necessário, controlada e/ou minimizada.

Os autores deste artigo, cuja experiência em Estudos Acústicos de Parques Eólicos e de aerogeradores é significativa e consistente, apresentam as metodologias seguidas na análise dos efeitos observados no ruído ambiente da zona de implantação de um Parque Eólico, bem como a especificação otimizada das características dos aerogeradores, em 2 artigos subordinados ao tema: *Parques Eólicos - Estudo dos Impactes no Ambiente Sonoro: I) Influência no Ruído Local; II) Configuração Otimizada de Potências Sonoras.*

No primeiro artigo (*I - Influência no Ruído Local*), é mostrado como o ruído gerado num Parque Eólico pode influenciar o ambiente sonoro da zona envolvente.

Neste segundo artigo (*II - Configuração Otimizada de Potências Sonoras*), é apresentada a metodologia seguida para minimizar os acréscimos de ruído no ambiente local devido às emissões acústicas dos diferentes aerogeradores.

Esta minimização passa por, inicialmente, construir um modelo 3-D do Parque Eólico, com todos os aerogeradores implantados no terreno. O modelo inclui os dados relativos aos terrenos e ao edificado bem como às potências sonoras das turbinas. A solução a implementar para a configuração mais favorável das potências sonoras de cada um dos aerogeradores, no sentido de garantir a menor perturbação no ambiente sonoro local, nomeadamente, nos locais com usos do solo com sensibilidade ao ruído existentes na sua proximidade, é encontrada através de métodos previsionais recursivos, que são descritos no artigo.

São apresentados os critérios subjacentes à optimização atrás referida, nomeadamente os constantes no Regime Legal sobre a Poluição Sonora, Anexo ao Decreto-Lei nº 292/2000 de 14 de Novembro - Critério de Exposição Máxima (classificação acústica de zonas) e Critério de Incomodidade.

#### Publicado em:

*Proceedings do Congresso Internacional ACÚSTICA 2004, Guimarães, Portugal, Setembro de 2004.*

# HERTZ CONTACT IN CHAIN ELASTIC COLLISIONS

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A theoretical analysis of the influence of the Hertz elastic contact on a three body chain collision is presented. Despite the elastic character of the collision, the final velocity of each particle depends on the interaction between them. Two elastic spheres falling together, one on top of the other under the action of gravity, and then colliding with the ground, are studied in detail.

**Publicado em:**

*American Journal of  
Physics, Vol. 72, 1488,  
2004.*

# MAGNETIC FORCES ACTING ON RIGID CURRENT-CARRYING WIRES PLACED IN A UNIFORM MAGNETIC FIELD

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We calculate the forces acting on segments of rigid wires carrying constant currents and placed in a uniform magnetic field. This example entices the students to formulate, explore and prove a conjecture, exposing them to an early example of a research-like project.

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*The Physics Teacher*  
42, 161, 2004.

07

# MATEMÁTICA

Anuário Científico 2004

ISEL



# CURRENT-PRESSURE CHARACTERISTICS OF PLANAR MAGNETRON DISCHARGES IN RARE GASES.

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The variation of current intensity with pressure, at constant voltage, ( $I$ - $p$  characteristics), was obtained for planar magnetron discharges in neon, krypton, and xenon on a copper target. The analysis of those curves confirms that an equation of the same type as the one recently obtained by the authors for an argon-copper discharge is an adequate relation to describe the dependence of current intensity on pressure and voltage for planar magnetron discharges in rare gases. That equation accounts for a bimodal behaviour corresponding to the sum of a “magnetron term” and a “diode term”.

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*Journal of Vacuum, Science & Technology A: Vacuum, Surfaces and Films* -22, 6 (2004) 2361-2364

# IFS WITH OVERLAPS AND HAUSDORFF DIMENSION

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*Grazer Mathematische  
Berichte 346 (2004)  
355-376*

We study IFS (iterated function systems) with overlaps and describe a procedure for computing the exact Hausdorff dimension of their attractor, giving an explicit formulae. The method introduced depends on the totally disconnected IFS's associated. We define the topological entropy for an IFS with overlaps. We introduce a class of Markov subshifts, which are designated by fractal Markov subshifts, using a weighted transition matrix, whose entries are Hausdorff dimension dependent. Therefore the fractal metric entropy and the fractal Lyapunov exponent are characterized with respect to a fractal Markov measure.

# WEIGHTED KNEADING THEORY OF ONE-DIMENSIONAL MAPS WITH A HOLE

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The purpose of this paper is to present a weighted kneading theory for one-dimensional maps with a hole. We consider extensions of the kneading theory of Milnor and Thurston to expanding discontinuous maps with holes and introduce weights in the formal power series. This method allows us to derive techniques to compute explicitly the topological entropy, the Hausdorff dimension and the escape rate.

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*International Journal of  
Mathematics and  
Mathematical Sciences*  
38 (2004), 2019-2038.

# COMPUTING TOPOLOGICAL AND METRICAL INVARIANTS

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*Proceedings of  
Dynamical Systems  
and Applications, 5-10  
Julho 2004, Antalya,  
Turquia.*

We study the dependence of the attractors on the contraction ratios of the iterated function systems, associated to expanding discontinuous maps with holes on the interval. For this class of maps, an extension of Milnor-Thurston theory is provided. Introducing weights on the formal power series, we establish a weighted kneading theory. We show that this method allow us to derive techniques to compute explicitly some topological and metrical invariants: the topological entropy, the Hausdorff dimension and the escape rate.

# HOW TO IMPROVE RETRIEVAL EFFECTIVENESS ON THE WEB?

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We explore the question of combining link analysis, content analysis and classification-based techniques to improve retrieval performance on the Web. We show the potential of fusion and that relatively simple implementation of combination does improve the retrieval performance.

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*E-Society 2004*  
<<http://www.iadis.org/e52004/>> , Avila (Spain)  
– 16th to 19th July  
2004.

# DOES OVERLAP MEAN RELEVANCE?

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The work developed in this paper focuses on the overlap of relevant retrieved documents obtained from different combination of systems and components. Study of the impact on information retrieval systems performance is also carried out.

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at Proceedings of  
WWW/Internet 2004  
pags. 877-900 (ISBN-  
972-99353-0-0)  
<[http://www.iadis.org/ic  
wiz2004/](http://www.iadis.org/ic<br/>wiz2004/)> (Madrid – 6th  
to 9th October 2004):*

# INFRAESTRUTURA MODULAR DE TESTE PARA PESQUISA DE INFORMAÇÃO.

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É abordado o problema da pesquisa de informação, nos diferentes modelos existentes, dando ênfase à construção de uma plataforma modular flexível, capaz de testar de uma forma controlada diferentes modelos de pesquisa e assim contribuir para o desenvolvimento do tema, evitando assim a construção de diferentes sistemas de pesquisa que seria necessário desenvolver para testar os diferentes modelos.

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*Proceedings of Ibero-  
Americana  
WWW/Internet 2004 <  
http://www.iadis.org/ci  
awi2004/> (Madrid –  
7th to 8th October  
2004):*

# COMBINAÇÕES DE SISTEMAS DE PESQUISA DE INFORMAÇÃO

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O presente trabalho explora o problema da pesquisa de informação na Web, explorando a combinação de resultados dos principais sistemas de pesquisa (textual, seguimento de ligações e classificação) de forma a melhorar os resultados da pesquisa de informação (i.e., aumento da precisão e cobertura). São analisados resultados das diferentes fórmulas de combinação tendo como objectivos a melhoria de resultados.

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Americana  
WWW/Internet 2004 <  
http://www.iadis.org/ci  
awiz2004/> (Madrid –  
7th to 8th October  
2004):*

# THE ACTIAS SYSTEM: SUPERVISED MULTI-STRATEGY LEARNING PARADIGM USING CATEGORICAL LOGIC

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One of the most difficult problems in the development of intelligent systems is the construction of the underlying knowledge base. As a consequence, the rate of progress in the development of this type of system is directly related to the speed with which knowledge bases can be assembled, and on its quality. We attempt to solve the knowledge acquisition problem, for a Business Information System, developing a supervised multi-strategy learning paradigm. This paradigm is centred on a collaborative data mining strategy, where groups of experts collaborate using data-mining process on the supervised acquisition of new knowledge extracted from heterogeneous machine learning data models.

The Actias system is our approach to this paradigm. It is the result of applying the graphic logic based language of sketches to knowledge integration. The system is a data mining collaborative workplace, where the Information System knowledge base is an algebraic structure. It results from the integration of background knowledge with new insights extracted from data models, generated for specific data modelling tasks, and represented as rules using the sketches language.

**Publicado em:**

*Ickeds'04, International Conference on Knowledge Engineering and Decision Support Proceedings, Porto 2004, 175-183.*

# LEARNING WITH INNER PRODUCT NETWORKS

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A new type of supervised neural networks, called Inner Product Networks, is proposed for supervised learning problems. The model is inspired by an initialization method for the weights of a multilayer perceptron (MLP) proposed by Denoeux [4] and building on the relation between the euclidean distance of two vectors and their inner product. We design an alternative model with the capability of local detection, as in radial basis function networks (RBFN) and with the capability of global influence over the entire input training space, as in MLPs. The model consists of a linear combination of basis functions,  $f_j$ ,  $f_j(x_i) = \tanh(-\alpha(x_i - c_j))$ , with  $\alpha$  playing a regularization role similar to that of the so-called temperature hyper parameter in sigmoidal activation functions, and  $c_j$  having a role similar to the centres of RBFNs. The training procedure is described and we analyse the application to three experiments with synthetic data.

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*Proceedings of the International Conference – Mathematical Methods for Learning, Como, Italy - 21st to the 24th June 2004.*

# ONLINE LEARNING WITH INNER PRODUCT NETWORKS

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The only essential difference between multilayer perceptrons (MLP) and radial basis function networks (RBFN) is that while one is based on the application of sigmoidal activation functions to inner products, the other is based on the application of kernel functions to euclidean distances. Building on the relation between the euclidean distance between two vectors and their inner product, we seek to design an alternative model with the capability of local detection, as in RBFNs, with the capability of global influence over the entire input training space, as in MLPs.

This work describes a new type of supervised neural networks called Inner Product Networks (IPN). The model consists of a linear combination of basis functions,  $f_j$ , each one associated to one of the input patterns,  $X_j$ :  $f(X_i) = \tanh(k(1 - X_i X_j))$ . The model is inspired by an initialization method for the weights of a MLP proposed by Denoeux [2]. We demonstrate the key role of the hyperparameter  $k$  with some artificial problems and we extended the use of these networks to online learning problems. The estimation of the linear parameters in the model is carried out through the Recursive Least Squares method. The number of units and the value of  $k$  can then be made variable, using appropriate heuristics.

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# A E-LEARNING COMO POTENCIADORA DE APRENDIZAGEM DISTRIBUÍDA

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A Internet e o papel que através da World Wide Web desempenha na transmissão de informação, é cada vez mais relevante principalmente pela flexibilidade e independência que proporciona a quem aprende. Existem diversas instituições de ensino superior que começam a utilizar este meio de comunicação como meio de distribuição dos conteúdos dos cursos que ministram. No entanto, a aprendizagem electrónica (a e-learning) não deve ser apenas definida como um novo meio de distribuição da informação aos alunos. Desenvolver programas/cursos através da Internet, com êxito, é uma tarefa difícil. Não se trata, apenas, de um problema de transposição das aulas tradicionais para um novo meio, mas de rentabilizar as possibilidades abertas pelas Tecnologias de Informação e Comunicação (TIC), de modo a conceber, implementar e avaliar o ensino e, mais importante, a aprendizagem. Nesta comunicação iremos apresentar o desenvolvimento e aplicação de um sistema de e-learning onde é possível ultrapassar as fronteiras da educação a distância e da educação presencial. O que se pretende é tirar o máximo proveito dos dois sistemas de ensino (presencial e a distância), repensando os conceitos de ensino e aprendizagem e tirando partido das novas possibilidades abertas pelas TIC. O sistema que está a ser desenvolvido pela Área Científica de Matemática do ISEL não se limita a “digitalizar” as aulas existentes e a disponibilizá-las na Internet. Tem como objectivos principais potenciar a aprendizagem activa, promover a reflexão e a produção e permitir que o Professor desempenhe o seu papel de orientador, facilitador e observador das aprendizagens, podendo de algum modo ultrapassar as barreiras impostas pelos factores tempo e distância.

O desenvolvimento do sistema tem as seguintes orientações pedagógicas:

- O centro do sistema deve ser a aprendizagem do estudante e não o ensino ou o Professor;
- A Aprendizagem deve alicerçar-se em conhecimentos estruturados, construídos por meio da acção, da comunicação e da reflexão;
- A reflexão é o ingrediente fundamental do sistema e deve ser estimulada, por meio de debates, bem como através de outros modos de representar o conhecimento (utilização de hipertexto, imagens,

som, gráficos, vídeo, etc.);

- O Professor é concebido como planificador, guia e observador; aquele que promove e facilita a aprendizagem;

- Os erros dos estudantes não devem ser evitados e ignorados, mas sim detectados para análise e discussão.

# MEMÓRIA LONGA DA VOLATILIDADE NO MERCADO DE CAPITAIS PORTUGUÊS

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Depois do trabalho de Engle, os modelos de heteroscedasticidade condicionada, vulgarmente designados por modelos tipo ARCH, têm sido utilizados na modelação da volatilidade das taxas de rendibilidade dos activos financeiros. No modelo GARCH, e quando a frequência dos dados é elevada, tem-se verificado que a soma das estimativas para os parâmetros está muito próxima da unidade, sugerindo uma elevada persistência na volatilidade, e tendo contribuído para o desenvolvimento de modelos de memória longa.

Neste trabalho, analisamos as características da volatilidade do mercado de capitais português, testamos a existência de memória longa nessa volatilidade e modelamo-la, recorrendo para tal ao modelo LMSV (Long Memory Stochastic Volatility). É ainda nosso propósito comparar a bondade do ajustamento entre este modelo e três outros vulgarmente designados por modelos de memória curta: GARCH, EGARCH e GJR. A inclusão dos dois últimos justifica-se pelo efeito assimétrico na volatilidade que caracteriza geralmente os mercados de capitais mais desenvolvidos.

# PREHEATING FOR FIELD INTERACTIONS OF A GENERAL FORM

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We consider the pre-heating mechanism for field interactions of a general form. Dealing with the corresponding perturbative equations requires an extension of the methods developed for the case  $\phi^2 \chi^2$ , where  $\phi$  is the inflaton field and  $\chi$  the matter field. We discuss the qualitative and quantitative features of different scenarios, both in the narrow and in the broad resonance regimes.

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# DINÂMICA DE MODELOS COSMOLÓGICOS

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