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ISEL

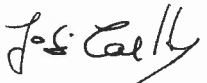
NOTA INTRODUTÓRIA

Com o anuário referente ao ano 2006 é completado um ciclo iniciado pelo Conselho Científico do Instituto Superior de Engenharia de Lisboa no ano de 2002 com a publicação do primeiro anuário científico do ISEL.

As vicissitudes na publicação da 6ª edição do Anuário Científico do ISEL, reflectem-se no atraso da sua saída. A implementação do processo de Bolonha, a reestruturação e criação de novos cursos em áreas emergentes do conhecimento e toda actividade implícita, para além de outros factores, ocasionou que me coubesse a concretização da edição deste anuário, ainda concluído pelo anterior Presidente do Conselho Científico, Professor Elmano Margato.

Acredito que a divulgação do conhecimento resultante da Ciência, Investigação e actividade profissional de mérito reconhecido são indissociáveis e insubstituíveis para uma Escola que lecciona cursos de Engenharia e se afirmou no panorama nacional e internacional.

O Presidente do Conselho Científico



(Prof. José A. Paixão Coelho)


01

ENGENHARIA CIVIL

Anuário Científico 2006

ISEL

A NON-DESTRUCTIVE METHOD FOR TESTING NON-FLEXIBLE DUAL GEOMEMBRANE SEAMS USING GAS PERMEATION

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A non destructive test is proposed to control in situ non-flexible geomembrane seams carried out by means of the thermal hot dual wedge method. It consists in pressurizing the gap between the two welds by gas injection at a specific pressure and in monitoring the evolution of pressure over time. The migration of gas across the géomembrane is indicated by a decrease in pressure. A permeation parameter (the time constant) can then be estimated under unsteady-state conditions. Experiments were performed outdoors, under variable ambient conditions to test the feasibility of the method in field conditions as well as in the laboratory, and under controlled ambient conditions to check the validity of the method. The results show that a poor seam from a mechanical point of view is also a poor seam from a permeation point of view. It is also shown that the non-destructive method presented here may be used in situ to test the entire seam. Hence the test is complementary to peel tests, because it reveals poor seams undetectable by the pressurized dual seam method, in pond applications where non-flexible géomembranes are placed.

Publicado em:
Revista Geosynthetics International, volume 13, nº 1, Janeiro de 2006.

ANÁLISE DOS MÉTODOS DE CONTROLO DE INTEGRIDADE DE GEOMEMBRANAS DE PEAD USADAS EM ATERROS DE RSU

Lopes, M.G.

ISEL, Lisboa, Portugal

Publicado em:
Revista Geotecnia nº 106, Março de 2006

Nos aterros de resíduos sólidos urbanos (RSU), as geomembranas são utilizadas no sistema de confinamento da base e taludes, como barreira à fuga de lixiviados, devendo resistir a agressões químicas e biológicas por parte dos resíduos, lixiviados e biogás, a agressões mecânicas durante a construção (tráfego de obra, colocação de camadas sobrejacentes, etc.) e exploração (peso dos resíduos, assentamentos da fundação, etc.) e ao efeito da exposição aos raios solares, entre outros. Como a eficácia do funcionamento do sistema de confinamento dos aterros de RSU está muito dependente do desempenho das geomembranas e este da sua integridade física, considerou-se importante apresentar os possíveis tipos e origens dos danos a que as geomembranas podem ser sujeitas e fazer uma análise dos métodos mais adequados para a detecção de orifícios e subsequente reparação.

A EXPERIÊNCIA DE COLOCAÇÃO DE GEOMEMBRANAS DE PEAD EM ATERROS DE RSU

Lopes, M.G.

ISEL, Lisboa, Portugal

Em Portugal, nos últimos 10 anos, houve uma grande mudança na política de gestão de resíduos, tendo-se encerrado as lixeiras existentes e construído em sua substituição cerca de 40 aterros de RSU. Numa altura em que os primeiros destes aterros começam a atingir o limite da sua vida útil, sendo por isso necessário iniciar uma nova fase de construções deste tipo de infra-estruturas e dada a importância que o desempenho das geomembranas tem na eficácia do funcionamento dos sistemas de confinamento dos aterros de RSU, considerou-se importante retirar alguns ensinamentos para o futuro sobre a experiência de colocação de geomembranas na base e taludes de mais de uma dezena de aterros de RSU do nosso país, nomeadamente no que respeita aos materiais utilizados, às técnicas empregues e aos problemas encontrados.

Publicado em:
Revista Geotecnia nº 106, Março de 2006. .

01

SISTEMAS DE IMPERMEABILIZAÇÃO E DRENAGEM DE TÚNEIS: SUA CONSTITUIÇÃO E TIPOLOGIAS

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Publicado em:
Revista Construção Magazine nº 15, 1º trimestre de 2006.

Muito embora a construção de obras subterrâneas seja muito antiga, a preocupação efectiva com a sua impermeabilização é bastante mais recente. Até à década de 1960, a impermeabilização era conseguida através do betão estrutural e da aplicação de injecções de caldas impermeabilizantes, quando as infiltrações surgiam. Contudo, muitas vezes estas medidas não eram suficientes, tendo de se recorrer a soluções mais onerosas, que passavam em muitos casos pela captação e condução da água. Começaram então a surgir obras com sistemas de impermeabilização contínuo, utilizando-se para o feito geomembranas, de custo inicial pouco relevante (da ordem dos 2%), mas que se traduziam numa economia significativa em termos de custos globais, por contribuírem para uma maior durabilidade da obra ao longo da sua vida útil e para a longevidade em boas condições de funcionalidade.

Em Portugal, só há cerca de uma década é que grande parte das obras subterrâneas é contemplada com um sistema de impermeabilização contínuo. Tendo em consideração que os conhecimentos sobre estes sistemas têm sido pouco divulgados, julgou-se oportuno neste artigo descrever a constituição destes sistemas e apresentar uma síntese das diferentes tipologias em função dos diversos processos construtivos.

OS GEOTÊXTEIS E A MARCAÇÃO CE

Lopes, M.G.

ISEL, Lisboa, Portugal

A aplicação de normas harmonizadas no âmbito dos geotêxteis e produtos relacionados está em vigor desde 2001, tendo a Comissão Europeia estabelecido a data de 1 de Outubro de 2002 para a obrigatoriedade da marcação CE destes produtos para a sua comercialização no espaço económico europeu. Neste artigo e após uma síntese dos princípios em que se baseia a marcação CE e das suas vantagens e implicações, referem-se os trâmites necessários para a obtenção da marcação CE para o caso particular dos geotêxteis e produtos relacionados, fazendo-se alusão nomeadamente às normas harmonizadas sobre estes produtos (destacando a sua estrutura base e os requisitos nelas contidos), ao sistema de comprovação de conformidade e aos organismos responsáveis por essa comprovação.

Publicado em:
Revista Construção Magazine nº 15, 1º trimestre de 2006.

01

METODOLOGIA DE ENSAIO DE JUNTAS DE SOBREPOSIÇÃO EM MEMBRANAS PREFABRICADAS DE IMPERMEABILIZAÇÃO

Gonçalves, M.[1]; Brito, J. de[2]; Grandão Lopes[3]; Lopes, M.G.[1]

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3 LNEC, Lisboa, Portugal

Publicado em:
Revista da APAET nº 12, 2006.

O desempenho dos revestimentos de impermeabilização de coberturas em terraço está muito dependente do comportamento das respectivas juntas de sobreposição. Com o objectivo de analisar esse comportamento sob a acção do vento, é feita uma descrição dos ensaios de tracção-corte e de pelagem a que as juntas são normalmente submetidas.

REVESTIMENTOS DE IMPERMEABILIZAÇÃO DE COBERTURAS EM TERRAÇO. FIXAÇÃO MECÂNICA

Gonçalves, M.[1]; Brito, J. de[2]; Grandão Lopes[3]; Lopes, M.G.[1]

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3 LNEC, Lisboa, Portugal

O desempenho de uma cobertura em terraço, relativamente aos agentes atmosféricos que nela actuam, é fortemente condicionado pelo seu sistema de impermeabilização. Sendo cada vez mais frequente a utilização de um sistema constituído por membranas de impermeabilização pré-fabricadas fixadas mecanicament, o presente artigo pretende divulgar as soluções de concepção e constituição deste tipo de sistemas capazes de conferirem um bom desempenho às coberturas em terraço.

Publicado em:
Revista Engenharia Civil e Vida nº 20, Janeiro de 2006.

ACCEPTANCE CRITERIA FOR HDPE GEOMEMBRANES DOUBLE HOT WEDGE SEAMS: THE INFLUENCE OF THE TEMPERATURE ON PEEL STRENGTH

Lopes, M.G.[1]; Barroso, M.[2]; Costa, C.[1]

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Publicado em:
Actas do "8th Internacional Conference on geosynthetics", Yokohama, Japão, 18 a 22 de Setembro de 2006.

In landfills, the decision of conformity/non-conformity of HDPE geomembranes double hot wedge seams is usually evaluated by destructive tests: peel and shear tests. Laboratory tests were conducted to study the influence of the temperature on peel strength of the seams. Eleven temperatures, ranging from 4 to 36 ºC, were considered. Two samples of HDPE geomembrane seams were used. For each temperature, both peel strength value and mode of rupture were recorded. Based on the results obtained, some correlations between peel strength and temperature values are proposed. As in the field it is not always easy to guarantee the accomplishment of the tests at the standardised temperature these correlations are very important to support the right decision of acceptance or rejection of the field seams.

PROBLEMES LIES A LA MISE EN PLACE DE GEOSYNTHETIQUES DANS DES CENTRES DE STOCKAGE DE DECHETS MENAGERS PORTUGAIS

Lopes, M.G.

ISEL, Lisboa, Portugal

Un important effort a été entrepris au Portugal au cours de ces dix dernières années afin d'adopter une nouvelle politique de gestion des déchets ménagers. Deux cents cinquante six décharges à ciel ouvert ont été progressivement fermées alors que dans le même temps environ quarante centres de stockage de déchets ménagers ont été construits. Dans ces ouvrages les géosynthétiques ont joué un rôle très important mais ont nécessité de recourir à de nouvelles approches au niveau du projet et de la construction. Cette communication a pour objectif de présenter les problèmes les plus fréquents qui ont été rencontrées au cours de la fermeture des décharges à ciel ouvert et de celles liées à la mise en place des géosynthétiques lors de la construction des centres de stockage de déchets ménagers portugais.

Publicado em:
Actas dos Rencontres 06–Geosynthetiques, Montpellier, França, 12 a 14 de Junho de 2006.

AVALIAÇÃO DO DESGASTE DE LOS ANGELES DE AGREGADOS A PARTIR DE ENSAIOS EM ROCHA

Conde, M.C.[1]; Lopes, M.G.[1]; Dinis da Gama, C.[2]

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Publicado em:
Actas do 10º Congresso Nacional de Geotecnia, Lisboa, 22 a 25 de Maio de 2006.

Neste artigo foram estabelecidas correlações entre as propriedades das rochas e dos agregados obtidos a partir destas, com o objectivo de estimar a aplicabilidade dos agregados, em camadas de base e sub base de infraestruturas rodoviárias, a partir de ensaios realizados sobre o material rochoso. Tendo em vista o objectivo do trabalho foi efectuada a caracterização mecânica dos materiais rochosos através da realização de ensaios de carga pontual e martelo de Schmidt e a cacterização mecânica dos agregados através da realização do ensaio de Los Angeles. Com os resultados obtidos, não só nos ensaios atrás referidos, mas também em resultados indicados por outros autores, foram estabelecidas correlações entre a resistência à compressão uniaxial (determinada a partir da dureza de Schmidt) e a resistência à carga pontual da rocha mãe, com o desgaste de Los Angeles dos agregados.

APLICAÇÃO DE IMPLEMENTAÇÃO NUMÉRICA DO TEOREMA CINEMÁTICO À DETERMINAÇÃO DE IMPULSOS DE TERRA

Asciuto, A.[1]; Antão, A.[2]; Guerra, N.[3]; Lopes, M.G.[1]

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Neste trabalho apresenta-se um estudo cujo objectivo principal é a aplicação e validação de um programa de cálculo automático que implementa numericamente o teorema cinemático à determinação dos valores dos coeficientes de impulso de terras sobre uma estrutura de suporte.

Os casos estudados correspondem a maciços puramente atríticos, com superfície horizontal, aplicando os impulsos sobre um paramento vertical rugoso. Determinam-se coeficientes de impulso correspondentes a carregamentos motivados pelo peso do solo e pela aplicação de sobrecargas à superfície do terreno. Comparam-se os valores obtidos e conclui-se sobre a validade da aplicação do princípio da sobreposição à consideração conjunta dos dois tipos de carregamento. Confrontam-se os valores calculados com os obtidos de soluções existentes do teorema cinemático e do teorema estático.

Publicado em:
Actas do 10º Congresso Nacional de Geotecnia, Lisboa, 22 a 25 de Maio de 2006.

IMPERMEABILIZAÇÃO DE TÚNEIS COM GEOMEMBRANAS

Justo, J.[1]; Lopes, M.G.[2]; Brito, J. de[3]

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Publicado em:
Actas do 10º Congresso Nacional de Geotecnia, Lisboa, 22 a 25 de Maio de 2006.

Exigências crescentes de funcionalidade, longevidade e segurança dos túneis levaram a que, na última década, se tenha recorrido cada vez mais em Portugal à sua impermeabilização contínua. Os sistemas de impermeabilização contínua e drenagem associada são normalmente constituídos por geossintéticos, pela sua grande adaptabilidade aos diferentes tipos de suporte, facilidade e rapidez de instalação, e boa relação qualidade/custo. Tendo em consideração a crescente utilização de sistemas de impermeabilização e drenagem associada (SImDA) de túneis com geossintéticos e simultaneamente a sua escassa divulgação, julgou-se oportuno apresentar neste artigo uma síntese dos diferentes tipos destes sistemas utilizados em túneis portugueses, os requisitos a serem observados na sua concepção e as respectivas metodologias de instalação.

CRITÉRIO DE ACEITAÇÃO/REJEIÇÃO DE SOLDADURAS POR TERMOFUSÃO DE GEOMEMBRANAS EM PEAD: A IMPORTÂNCIA DA TEMPERATURA DE ENSAIO

Lopes, M.G.; Costa, Carla

ISEL, Lisboa, Portugal

A resistência mecânica das soldaduras por termofusão de geomembranas em PEAD é normalmente determinada através de ensaios destrutivos de arranque (peel test) e de corte (shear test). É com base nos resultados destes ensaios que em obra se verifica a conformidade/não conformidade da soldadura relativamente à sua resistência. Neste artigo mostra-se como a temperatura de realização dos ensaios de arranque e de corte influencia os seus resultados e alerta-se para as consequências que pode ter na decisão de rejeição/aceitação das soldaduras.

Publicado em:
Revista Geotecnia nº 109, Novembro de 2006.

ESCÓRIAS DE R.S.U.: CARACTERIZAÇÃO MECÂNICA PARA FINS RODOVIÁRIOS

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Publicado em:
Livro de Resumos do 10.º Congresso Nacional de Geotecnia, Lisboa, Portugal, Maio de 2006

Neste trabalho são estudadas as propriedades mecânicas, tais como a rigidez e a resistência, de escórias provenientes da incineração de resíduos sólidos urbanos na incineradora da Valorsul, S.A.. Pretende-se avaliar, sob o ponto de vista geotécnico, a viabilidade de utilização deste material alternativo nas camadas estruturais de pavimentos rodoviários. Neste sentido, são apresentados resultados provenientes dos seguintes ensaios laboratoriais: análise granulométrica; ensaios C.B.R. e ensaio triaxial estático consolidado não drenado com medição das pressões intersticiais. Este estudo pretende contribuir para a valorização das escórias, cuja produção em Portugal, para 2006, se estima em cerca de 293 000 toneladas por ano. Para além de permitir reduzir a quantidade de resíduos a encaminhar para deposição final, o estudo também implica a diminuição da exploração de agregados naturais.

MODELAÇÃO BIDIMENSIONAL DE ANCORAGENS EM ESCAVAÇÕES SUPORTADAS POR ESTRUTURAS DE CONTENÇÃO FLEXÍVEIS

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Recorre-se em Portugal, de forma quase generalizada, à utilização de ancoragens para a realização de escavações em meio urbano suportadas por estruturas de contenção flexíveis. A análise destas estruturas de suporte passa, em muitos casos, pela realização de análises numéricas tensão-deformação, recorrendo geralmente ao método dos elementos finitos. Muitas destas análises são realizadas em condições bidimensionais, assumindo com frequência a validade do estado plano de deformação. As ancoragens, como elementos lineares que impõem, na zona de selagem, importantes efeitos tridimensionais, apresentam algumas dificuldades de modelação que têm sido abordadas por diversos autores. Apresentou-se neste trabalho as diferentes metodologias de modelação bidimensional de ancoragens e realizou-se um estudo comparativo dos resultados da sua aplicação, discutindo as suas vantagens e inconvenientes.

Publicado em:
Livro de Resumos do 10º Congresso Nacional de Geotecnia, Lisboa, Portugal, Maio de 2006

SOBRE AS FONTES DO TSUNAMI DE 1755: RESULTADOS PRELIMINARES DA PROPAGAÇÃO NO ESTUÁRIO DO TEJO

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Publicado em:
10ª Conferencia Nacional de Geotecnia, Lisboa, Portugal, 2006

O tsunami gerado pelo sismo de 1 de Novembro de 1755 é um dos eventos históricos melhor documentados. A discussão da localização e do mecanismo que lhe deu origem é ainda uma questão em aberto porque até agora nenhuma das soluções propostas explica de forma satisfatória o conjunto de observações do tsunami e as intensidades macrosismicas deduzidas dos relatos históricos. Neste trabalho apresenta-se uma comparação, para o tsunami, das soluções propostas mais importantes: a solução Marquês de Pombal/Banco do Guadalquivir e a solução zona de subducção no Golfo de Cadiz. O impacto no estuário do Tejo de um fenómeno semelhante a 1755, teria hoje diferentes consequências uma vez que a costa se encontra densamente povoada. Apresentam-se aqui os resultados preliminares das zonas potenciais de inundação na região do estuário.

A AVALIAÇÃO DE TERRENOS URBANOS NO CONTEXTO DA QUALIDADE DA GESTÃO DE EMPREENDIMENTOS IMOBILIÁRIOS

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A avaliação de um terreno urbano é uma das peças de base na qualidade da gestão de um empreendimento imobiliário, uma vez que o conhecimento correcto do presumível valor do terreno, constitui um dado fundamental quer para o detentor do mesmo quando o pretende vender, quer para o investidor que o pretende adquirir, quer para a entidade bancária que irá financiar a operação.
Um terreno vale em função daquilo que nele se puder edificar, ou um conjunto de terrenos valem em termos médios, em função da área média que neles se puder edificar. Por isso, a estimação de valor para um terreno urbano ou urbanizável, não pode ser realizada por métodos expeditos ou de simples comparação. Tem sim que passar pela previsão da sua possível melhor ocupação futura, e a partir daí, por um estudo económico completo e ponderado com todas as variáveis passíveis de fazer alterar o seu valor e que seja o mais aderente possível à realidade futura.
A presente comunicação descreve e exemplifica as metodologias a seguir para a realização desse trabalho, fornecendo ao leitor as ferramentas essenciais para o poder executar.

Publicado em:
Livro de Actas do Encontro Nacional sobre Qualidade e Inovação na Construção, QIC2006, LNEC, 21 a 24 de Novembro de 2006

DIAPHRAGM WALLS – HOW THE PECK DIAGRAMS ALLOW GOOD PREDICTIONS IN WALL DESIGN

Matos e Silva, J.

Gapres, S.A./ISEL, Lisbon, Portugal

Publicado em:
Publicado na Revista do Deep Foundations Institute (DFI Magazine), edição "Summer 2004", editada em Janeiro de 2005

ABSTRACT

The author that designs diaphragm walls curtains for more than 30 years developed an elasto-plastic method to make more accessible to the students the structural and geotechnical behaviour of anchored diaphragm walls.

So the so-called "Simplified method" is based in the following assumptions:

- It considers as the most unfavourable phase the one that corresponds to the final excavation stage and to the prestressing of all anchors;
- It neglects the elastic displacement of the anchors of the diaphragm wall.

The first design step is to define the plastic earth pressures on the diaphragm wall curtain:

- active pressure on the back of the curtain;
- passive pressure in front of the curtain base.

The second design step is to evaluate the bending moments diagram of the curtain considered, in this stage, as a vertical cantilever with-out anchorages.

From the bending moments diagram and considering that each level of anchorages allows the condition $\Sigma M = 0$ at the depth of the immediate lower level of anchorages it is possible to quantify the needed prestress to be applied at each anchorage level.

The third design step is to quantify the elastic pressure on the soil due to the prestress in the anchorages. This quantification is made based on the so-called "Peck Diagrams".

Obtaining the elastic diagram for each level of anchorages it is then possible to make the addition of all diagrams so considering the interaction of all levels of anchorages.

The fourth design step is to over pose the "plastic pressures diagram" obtained in the first design step with the "elastic pressures diagram" of the third design step, so obtaining the "evolving pressures diagram" that, at each depth, quantifies the greater value from both referred diagrams.

The fifth and final design step consists in dimensioning the curtain assuming its behaviour as a continuous vertical beam acted by the "evolving pressures diagram".

A RETRACÇÃO DO BETÃO – COMO ATENUAR OS SEUS EFEITOS

Nunes, Ângela[1]; Gonçalves, Arlindo[2]; Bettencourt Ribeiro[3]; Esteves, Paulo[4]; Matos e Silva, J.[5]

1 Quadro da Secil
2 Investigador Coordenador do LNEC
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RESUMO

Este artigo pretende ser um resumo das conclusões da acção, com o mesmo título, realizada na sede da Ordem dos Engenheiros no dia 23/06/2004, com a intervenção dos signatários.

A retracção é um fenómeno que decorre da hidratação do ligante e da secagem do betão e que se traduz numa redução de volume das peças de betão simples ou armado. Se esta redução de volume for restringida, pode provocar tensões de tracção e conduzir ao aparecimento de fissuração com todos os inconvenientes decorrentes tanto do ponto de vista estético como da funcionalidade das estruturas.

É por isso importante conhecer correctamente a génese deste fenómeno para se poder intervir correctamente e assim, atenuar os seus efeitos.

A retracção consiste numa variação de volume duma peça de betão (simples ou armado) que, no caso de ser restringida pode provocar tensões de tracção mais ou menos elevadas com a consequente ocorrência de fissuração.

Publicado em:
Publicado na Revista da ATIC – Associação Técnica da Indústria do Cimento, nº 28, Maio de 2006

MONITORIZAÇÃO DO COMPORTAMENTO DUM MURO DE GABIÕES COM 13 m DE ALTURA

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Publicado em:
Publicado no 10º Congresso Nacional de Geotecnia, Lisboa, 2006

RESUMO

A comunicação refere o caso dum muro de suporte de gabiões, localizado em Belas, no perímetro da Central de Valorização Orgânica da Valorsul, a Norte desta, e sobranceiro à Estrada Nacional.

Após a execução do muro e depois da ocorrência de pluviosidade significativa, verificaram-se algumas situações anómalas como sejam o esmagamento de parte do seu material pétreo e a ocorrência de deformações excessivas.

Face a estas patologias o muro foi inspeccionado e detectou-se que o material pétreo era parcialmente constituido por elementos de calcário margoso que, sob a acção da água, perdiam a sua resistência mecânica.

O muro foi demolido, reconstruido com material pétreo adequado e instrumentado. Durante a execução do aterro de tardoz procedeu-se à observação do seu comportamento.

Apresentam-se os resultados obtidos e as correspondentes conclusões.

REABILITAÇÃO ESTRUTURAL COM RECURSO À MICROESTACAS

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RESUMO

A comunicação refere o caso dum edifício localizado na Av. 24 de Julho, nº 52, em Lisboa, que foi erigido no início do Século XX.

Na sequência de trabalhos de rebaixamento do nível freático promovidos na envolvente, apareceu fissuração abundante nas paredes divisórias dos pisos elevados do edifício. Essas paredes são paralelas às fachadas principal e de tardoz do edifício e as fissuras ocorreram na ligação às paredes de empena revelando que havia assentamentos diferenciais entre estas e as divisórias interiores.

Ao nível dos tectos apareceu, também, fissuração ao longo da ligação às paredes de empena. Como os pavimentos são de madeira e os barrotes estão colocados paralelamente às empenas, esta fissuração revelava que havia um movimento descendente das paredes divisórias em relação às empenas.

A monitorização das fissuras revelou que a abertura destas progredia ao longo do tempo.

Como as paredes divisórias são suportadas, ao nível do r/c, por arcos de alvenaria, e havia fissuras nesses arcos, tudo indiciava para que a origem das patologias estivesse relacionada com as fundações.

Foi decidido promover no local, uma prospecção geotécnica recorrendo à execução de poços de inspecção às fundações.

Foi assim possível detectar que as fundações das empenas e das nascenças dos arcos eram constituídas por blocos calcários de pequena e média dimensão, com argamassa pouco preservada e degradada, com cerca de 1,5 m de altura, apoiadas nos níveis miocénicos superficiais, de natureza argilosa, com reduzida capacidade de carga (valores de resistência dinâmica qd entre 1 e 3 MPa.

A partir da base dos poços executaram-se ensaios de penetrómetro dinâmico super-pesado (DPSH) utilizando um equipamento normalizado do tipo Nordmeyer.

Os resultados dos ensaios revelaram que os materiais miocénicos muito descomprimidos, sobre os quais se apoiam as fundações existentes do edifício, atingem profundidades da ordem dos 7 a 8 m. Estão sobrejacentes a uma formação miocénica com comportamento

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mecânico favorável, apresentando valores de qd superiores a 10 MPa. O nível freático foi detectado a cerca de 4 m de profundidade.

Face a este ambiente geotécnico, pareceu indubitável que a variação do nível freático na envolvente, relacionada com trabalhos de bombagem, seria responsável pelo assentamento da camada de solos descomprimidos.

A solução técnica adoptada para o problema em causa consistiu em:

- reforçar as fundações das nascenças dos arcos utilizando microestacas, de modo a transferir as cargas para uma formação mais profunda e de maior capacidade portante do que a dos solos descomprimidos que suportam as fundações existentes;
- executar tirantes de betão armado (betão da classe C20/25 e aço A 400 NR), ligando as nascenças de cada arco, ao nível do r/c, de modo a absorver as reacções horizontais na base dos arcos, resultantes das acções verticais transmitidas pelas paredes divisórias interiores dos andares superiores. Deste modo as microestacas terão de suportar apenas as acções horizontais devidas à actuação do vento e do sismo e, para esse efeito, foram executadas microestacas inclinadas de cerca de 10º com a vertical. Os tirantes foram ligados às fundações existentes através de ferrolhos selados com resinas epoxídicas a furos, ligeiramente inclinados com a horizontal, préviamente executados no interior dessas fundações.

As microestacas tiveram um comprimento médio de 12 m e foram furadas através da base dos arcos de modo a assegurar uma mais directa transferência de cargas.

Adoptaram-se, em cada uma das nascenças dos arcos confinantes com as empenas, três microestacas de capacidade unitária 500kN e diâmetro nominal de 127 mm (5”). Nas nascenças interiores executaram-se duas microestacas de capacidade unitária 1000kN e diâmetro nominal de 152 mm (6”).

Para as primeiras utilizaram-se tubos metálicos TM 80 Ø 88,9 x 7,5 mm e, para as segundas, tubos TM 80 Ø 122 x 9 mm.

Os tubos foram de aço com um limite elástico de 562,0 x 103 kN/m^2 e a injecção de calda foi efectuada com equipamento que permite um débito máximo de 6 m^3/h com uma pressão até 100 bar.

A nova monitorização efectuada, posteriormente à intervenção descrita, revelou a estabilização da fissuração ocorrida, comprovando que a solução de intervenção adoptada foi a adequada para resolver o problema em causa.

DIMENSIONAMENTO E PORMENORIZAÇÃO DAS ZONAS SUJEITAS À ACÇÃO LOCALIZADA DO PRÉ-ESFORÇO SEGUNDO O EC2

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Pretende-se com esta comunicação apresentar em linhas gerais as disposições do EC2 relativas ao dimensionamento e pormenorização das zonas sujeitas à acção localizada do pré-esforço por pos-tensão, com particular ênfase nos aspectos que são diferentes ou novos em relação ao REBAP.

Alguns aspectos são diferentes nos dois regulamentos, nomeadamente:

- Factor de segurança a aplicar à força transmitida pela ancoragem;
- Valor da tracção resultante da aplicação da carga concentrada;
- Valor máximo das tensões nas armaduras para efeitos de controlo de abertura de fendas.

Para além da discussão destes aspectos, far-se-á ainda uma breve descrição dos modelos correntemente utilizados na análise das zonas sujeitas a forças concentradas. A este respeito serão confrontados os modelos de elementos finitos e os modelos de bielas e tirantes, também conhecidos como modelos de campos de tensões.

Visto que a utilização destes últimos é claramente encorajada no EC2, serão apresentados vários modelos adequados à análise de diversos casos práticos.

Será também discutida a recomendação do EC2 relativa ao número máximo de acoplamentos a dispor numa mesma secção.

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CARBONATION AND CHLORIDE PENETRATION IN CONCRETE MADE WITH FINE RECYCLED CONCRETE AGGREGATES

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Fine recycled aggregates are the stepsons of recycling for concrete production. Many references quote their detrimental influence on the most important characteristics of concrete: compressive and tensile strength; modulus of elasticity; water absorption; shrinkage; carbonation and chloride penetration.

These two last characteristics are fundamental in terms of long-term durability of reinforced or prestressed concrete. In the experimental research performed at IST, different concrete mixes (with increasing rates of substitution of fine natural aggregates - sand - with fine recycled aggregates) were prepared and tested. The results were then compared with the corresponding values of a reference concrete, with exactly the same composition and grading curve, but with no recycled aggregates.

This paper presents the main results of this research concerning carbonation and chloride penetration (by means of chloride migration coefficient) and draws some conclusions on the viability of using this type of aggregates in structural concrete, taking into account the obvious positive environmental impact that may arise from it.

NUMERICAL SIMULATION OF AN OLDROYD-B FLUID WITH A PRECONDITIONED DOMAIN DECOMPOSITION METHOD

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This paper deals with the numerical implementation of a preconditioned domain decomposition method to approximate the solution of a non-Newtonian viscoelastic Oldroyd-B model. The governing equations can be decomposed into a Navier-Stokes system and a transport equation and a modified Schwarz scheme, involving block preconditioners for the Navier-Stokes equations, is used to solve iteratively the decoupled problems. Numerical results are provided for steady flow in the two-dimensional lid driven cavity.

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A PRECONDITIONED DOMAIN DECOMPOSITION METHOD FOR THE SIMULATION OF VISCOELASTIC FLOWS

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WSEAS -Transactions on MATHEMATICS, issue 3, vol. 5, pp. 289-296, 2006.

In this paper we apply a domain decomposition method to approach the solution of a non-Newtonian viscoelastic Oldroyd-B model. The numerical scheme is based on a fixed-point argument applied to the original non-linear system of partial differential equations decoupled into a Navier-Stokes system and a tensorial transport equation. Using a modified Schwarz algorithm, involving block preconditioners for the Navier-Stokes equations, the decoupled problems are solved iteratively. Numerical simulations on a 4:1 abrupt contraction flow problem are considered to validate the scheme.

METODOLOGIA DE ENSAIO DE JUNTAS DE SOBREPOSIÇÃO EM MEMBRANAS PREFABRICADAS DE IMPERMEABILIZAÇÃO

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Revista Mecânica Experimental APAET, n.º 12, Lisboal, Março de 2006, páginas 30-35.

A cobertura em terraço de um edifício, entendida como o conjunto de todos os elementos estruturais e intermédios desde o tecto à superfície exposta às intempéries, é constituída por um conjunto de camadas dispostas horizontalmente ou próximo desta posição, que, pela sua constituição, permitem dar satisfação às suas principais exigências funcionais. O suporte da impermeabilização (em geral a camada de isolamento térmico), o revestimento de impermeabilização e a sua protecção, contam-se entre as possíveis e principais camadas da generalidade das coberturas em terraço.

O revestimento de impermeabilização deve garantir que exigências de segurança, aptidão ao uso e conservação das qualidades sejam satisfeitas para que a cobertura em terraço tenha um bom desempenho.

Num revestimento de impermeabilização de camada única, a satisfação destas exigências funcionais é condicionada pela natureza das membranas de impermeabilização a aplicar, pela ligação destas ao suporte (quando essa ligação existe na zona corrente) e pela ligação das mesmas através das juntas de sobreposição.

No caso dos revestimentos de impermeabilização de camada única fixados mecanicamente, as membranas de impermeabilização devem satisfazer as especificações técnicas europeias pertinentes e as Directivas ou Guias da UEAtc aplicáveis.

Quanto às ligações entre membranas, através de juntas de sobreposição, estas devem ser concebidas e executadas de forma a impedirem toda e qualquer influência nefasta para o bom funcionamento do revestimento de impermeabilização.

Sendo diversos os parâmetros que intervêm no desempenho das juntas de sobreposição dos revestimentos de impermeabilização, é usual utilizar os ensaios de tracção-corte e de pelagem para se obter informação sobre a qualidade destas ligações.

Dos factores que condicionam o comportamento das juntas entre duas membranas de impermeabilização, uns estão relacionados com a própria natureza das membranas, outros com a concepção e execução das juntas e outros ainda com as condições ambientais a que os sistemas estão sujeitos. Estes factores podem causar diversos de-

feitos, tanto nas próprias membranas como nas suas juntas de sobreposição.
Estudos efectuados sobre os vários tipos de problemas que ocorreram em sistemas de impermeabilização de camada única mostraram que os mais comuns se relacionam com um mau comportamento das juntas de sobreposição das membranas.
Assim, foi objectivo principal deste artigo dar a conhecer os procedimentos a implementar em campanhas experimentais que tenham como objectivo conhecer o comportamento das juntas de sobreposição das membranas.

FIXAÇÃO MECÂNICA DOS SISTEMAS DE IMPERMEABILIZAÇÃO DAS COBERTURAS EM TERRAÇO

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O desempenho de uma cobertura em terraço, relativamente aos agentes atmosféricos que nela actuam, é fortemente condicionado pelo do seu sistema de impermeabilização.

Os materiais de impermeabilização de coberturas e os sistemas por eles constituídos são diversos e a sua classificação pode estabelecer-se segundo diferentes critérios: funcionalidade, natureza dos materiais, técnica de colocação em obra, tipo de armadura das membranas, carácter tradicional ou não e ainda quanto ao modo de ligação ao suporte, quanto à sua constituição e quanto à acessibilidade. Actualmente, em Portugal, são diversas as opções para os sistemas de impermeabilização de coberturas em terraço, começando a ter utilização crescente os sistemas formados por membranas prefabricadas fixadas mecanicamente. Para estes, interessa portanto conhecer as diversas soluções de fixação. Mas, porque estes sistemas apresentam algumas particularidades, têm surgido anomalias distintas das que se manifestam em outras soluções de revestimento de impermeabilização com outras formas de ligação ao suporte. Assim, também é conveniente conhecer os parâmetros a ter em conta na concepção deste tipo de sistemas de impermeabilização de modo a evitar ou a minimizar a ocorrência de possíveis anomalias.

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Revista Engenharia & Vida, Ano II n.º 20, Lisboa, Janeiro 2006, páginas 30-36.

01

IN SEARCH OF THE 31 MARCH 1761 EARTHQUAKE AND TSUNAMI SOURCE

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ABSTRACT

Earthquake catalogues for the Iberian Peninsula report three strong magnitude events in the XVIII Century: 27.12.1722, 1.11.1755, 31.03.1761. These events have magnitudes greater than 7 and generated tsunamis that damaged the Portuguese coasts. However, their source areas are controversial due to the lack of detailed and coherent historical descriptions.

The 31 March 1761 earthquake was felt in Lisbon at noon, alarming the inhabitants and throwing down ruins of the past 1st November 1755 earthquake. According to several sources the earthquake was followed by a tsunami that was observed as far as Cornwall (United Kingdom), Cork (Ireland) and Barbados (Caribbean). The Portuguese catalogues locate this event on the Horseshoe Abyssal Plain, south of Gorringe Bank and attribute a magnitude of 7.5. The Caribbean tsunami catalogue (Lander et al., 2002), locates the event further north 37ºN 10ºW and estimates of its epicenter intensity as IX.

In this study we present a reappraisal of the available historical reports concerning the 1761 event, a revision of the macro-seismic intensities along Iberia and the tsunami observations along the western Portuguese and Galicia coasts, England, Ireland and the West Indies. With this dataset we use backward ray tracing techniques to discuss the location of the event and its integration with one of the major tsunami generation areas in the western Portuguese margin. We conclude that 1761.03.31 earthquake took place at 12:01 am (Lisbon time). Its epicenter was located circa 34.5ºN 13ºW and had a tsunami magnitude close to 8.5.

TSUNAMI PROPAGATION ALONG TAGUS ESTUARY, LISBON – PORTUGAL (PRELIMINARY RESULTS)

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ABSTRACT

In this study we present preliminary results of flood calculation along Tagus Estuary, catastrophic event that happened several times in the past, as described in historical documents, and that constitutes one of the major risk sources for Lisbon coastal area. To model inundation we used Mader's SWAN model for the open ocean propagation with a 2 km grid, and Imamura's TSUN2 with a 50 m grid covering the entire estuary. The seismic source was computed with the homogeneous elastic half space approach. Modelling results agree with historical reports. Synthetic flood areas correspond to the sites where there are morphological and sedimentary evidences of two known major events that stroke Lisbon: 1531.01.26 and 1755.11.01 tsunamis.

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Science of Tsunami Hazards, Vol. 24, No. 5, page 329 (2006)

SOURCE OF THE 1693 CATANIA EARTHQUAKE AND TSUNAMI (SOUTHERN ITALY): NEW EVIDENCE FROM TSUNAMI MODELING OF A LOCKED SUBDUCTION FAULT PLANE

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The 1693 Catania earthquake, which caused 60000 deaths in eastern Sicily and generated a 5–10 m high tsunami, is investigated. GPS data indicate ESE-WNW convergence in the Calabrian arc at 4–5 mm/yr. New highresolution seismic data image active compression at the toe of the accretionary wedge. The lack of instrumentally recorded thrust earthquakes suggests the pre-sence of a locked subduction fault plane. Thermal modeling is applied to calculate the limits of the seismogenic zone. Tsunami modeling is performed to test the hypothesis that the 1693 earthquake occurred on the subduction fault plane (160–120 km in size) with 2 m of mean co-seismic slip. This source successfully reproduces historical observations with regard to polarity and predicts 1–3 m high amplitudes. It is likely that only the SW segment of the subduction fault plane ruptured in 1693 and 1169, implying a recurrence interval of roughly 500 years for similar events.

THE GIBRALTAR ARC SEISMOGENIC ZONE (PART 2): CONSTRAINTS ON A SHALLOW EAST DIPPING FAULT PLANE SOURCE FOR THE 1755 LISBON EARTHQUAKE PROVIDED BY TSUNAMI MODELING AND SEISMIC INTENSITY

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The Great Lisbon earthquake has the largest documented felt area of any shallow earthquake and an estimated magnitude of 8.5–9.0. The associated tsunami ravaged the coast of SW Portugal and the Gulf of Cadiz, with run-up heights reported to have reached 5–15 m. While several source regions offshore SW Portugal have been proposed (e.g. - Gorringe Bank, Marquis de Pombal fault), no single source appears to be able to account for the great seismic moment as well as all the historical tsunami amplitude and travel time observations. A shallow east dipping fault plane beneath the Gulf of Cadiz associated with active subduction beneath Gibraltar, represents a candidate source for the Lisbon earthquake of 1755. Here we consider the fault parameters implied by this hypothesis, with respect to total slip, seismic moment, and recurrence interval to test the viability of this source. The geometry of the seismogenic zone is obtained from deep crustal studies and can be represented by an east dipping fault plane with mean dimensions of 180 km (N–S)x210 km (E–W). For 10 m of co-seismic slip an Mw 8.64 event results and for 20 m of slip an Mw 8.8 earthquake is generated. Thus, for convergence rates of about 1 cm/yr, an event of this magnitude could occur every 1000–2000 years. Available kinematic and sedimentological data are in general agreement with such a recurrence interval. Tsunami wave form modeling indicates a subduction source in the Gulf of Cadiz can partly satisfy the historical observations with respect to wave amplitudes and arrival times, though discrepancies remain for some stations. A macroseismic analysis is performed using site effect functions calculated from isoseismals observed during instrumentally recorded strong earthquakes in the region (M7.9 1969 and M6.8 1964). The resulting synthetic isoseismals for the 1755 event suggest a subduction source, possibly in combination with an additional source at the NW corner of the Gulf of Cadiz can satisfactorily explain the historically observed seismic intensities. Further studies are needed to sample the turbidites in the adjacent abyssal plains to better document the source region and more precisely calibrate the chronology of great earthquakes in this region.

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Tectonophysics, 2006, doi:10.1016/j.tecto.2006.02.025. on line at www.sciencedirect.com

ESCÓRIAS DE R.S.U.: CARACTERIZAÇÃO MECÂNICA PARA FINS RODOVIÁRIOS

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Livro de Resumos do 10.º Congresso Nacional de Geotecnia, Lisboa, Portugal, Maio de 2006

Neste trabalho são estudadas as propriedades mecânicas, tais como a rigidez e a resistência, de escórias provenientes da incineração de resíduos sólidos urbanos na incineradora da Valorsul, S.A.. Pretende-se avaliar, sob o ponto de vista geotécnico, a viabilidade de utilização deste material alternativo nas camadas estruturais de pavimentos rodoviários. Neste sentido, são apresentados resultados provenientes dos seguintes ensaios laboratoriais: análise granulométrica; ensaios C.B.R. e ensaio triaxial estático consolidado não drenado com medição das pressões intersticiais. Este estudo pretende contribuir para a valorização das escórias, cuja produção em Portugal, para 2006, se estima em cerca de 293 000 toneladas por ano. Para além de permitir reduzir a quantidade de resíduos a encaminhar para deposição final, o estudo também implica a diminuição da exploração de agregados naturais.

BREVE APRESENTAÇÃO DA REUTILIZAÇÃO DE ÁGUAS RESIDUAIS EM PORTUGAL E NA UNIÃO EUROPEIA

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RESUMO

A presente comunicação resulta do trabalho desenvolvido pela Comissão Especializada de Águas residuais da APDA, especificamente o Grupo de Trabalho 3 - "Reutilização de Águas Residuais". Considera-se que o assunto em análise se reveste de especial importância e actualidade, na medida em que, face ao momento de "Seca Extrema" em que grande parte do nosso país se encontra, esta poderá ser uma forma viável de poupar as reservas de água existentes.

A abordagem que se efectuou não pretende divulgar qualquer tipo de tecnologia ou casos específicos, mas sim proporcionar uma partilha de experiências adquiridas pelas entidades que neste artigo participaram. O objectivo é sensibilizar e promover a reflexão sobre este assunto, de modo que, no futuro, os casos de sucesso de reutilização possam ser em maior número e de maior dimensão do que actualmente acontece.

Neste contexto, são identificadas alguns dos diferentes tipos de reutilização possíveis, os principais benefícios, os processos de tratamento e os requisitos de qualidade da água residual tratada necessários para algumas aplicações, bem como é apresentada uma breve análise do estado da arte tanto em Portugal, como em alguns países da União Europeia (UE).

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Tecnologia da Água, Nº 46, Portugal, Novembro/Dezembro de 2006.

CRACKING ANALYSIS IN CONCRETE DAMS USING ISOTROPIC DAMAGE MODELS. OBJECTIVITY OF NUMERICAL SOLUTIONS

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Livro de Resumos do III European Conference on Computational Mechanics, Solids, Structures and Coupled Problems in Engineering, LNEC, Lisboa, Portugal, Junho de 2002.

The numerical simulation of cracking in large concrete structures can be made, in many cases, adopting the smeared cracking approach and using constitutive laws of continuous damage (with softening), in order to simulate the material tension ruptures.
The consideration of a tension softening branch that depends on the value of the material fracture energy, implies the localization phenomena and requires the use of some specific numerical procedures in finite element analysis. Namely, consistent formulations evolving the energy dissipated during the rupture process must be used in order to obtain numerical results that do not dependent on the mesh discretisation – mesh objectivity.
In this paper, a 3D finite element formulation and a constitutive law of isotropic damage, with two independent variables, conceived to model the tension and compression softening effects (independently), are presented. The finite element model is used in the analysis of the Cabril Dam (the largest Portuguese arch dam) when submitted to the self-weight and the hydrostatic pressure (water at crest level). Numerical results related with the cracks propagation for dif-ferent 3D finite element discretisations are presented, in order to analyze the solutions objectivity. These results consist of (i) the radial displacements, (ii) the principal stresses and (iii) the tensile damages at the dam (i) central cantilever and/or (ii) upstream and downstream faces (Fig.1).

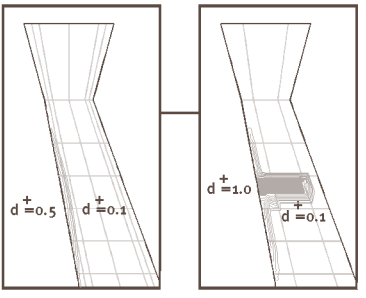

Figura 1 – Comparison of radial displacements and tensile damages for the two meshes.

SEGURANÇA RODOVIÁRIA ALGUMAS REFLEXÕES SOBRE METODOLOGIAS DE GESTÃO E SUA IMPLEMENTAÇÃO EM PORTUGAL

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Apresentam-se algumas reflexões sobre a utilização de abordagens metodológicas, suportadas em análise de matrizes de risco e custos sociais, como ferramentas a utilizar no apoio à gestão do investimento em segurança rodoviária. Faz-se uma breve introdução ao tema, na qual a Prevenção é evidenciada face às três componentes fundamentais dos sistemas de transportes: infra-estrutura, veículo e utilizador. De seguida, descrevem-se os principais conceitos associados à abordagem apresentada. Para uma melhor compreensão e objectividade a discussão é ilustrada com um pequeno exemplo relativo a uma intervenção num trecho do IP4, a partir da qual se percebe melhor o alcance e importância dos ganhos em eficácia e eficiência obtidos. Finalmente, tecem-se algumas considerações e apontam-se factores colaterais que não foram abordados, mas são fundamentais para uma viabilização das intervenções.

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DEVELOPMENT OF DAM FINITE ELEMENT MODELS FOR DYNAMIC ANALYSIS USING AMBIENT VIBRATION TEST RESULTS

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Publicado em:
Proceedings of III European Conference on Computational Mechanics, Lisbon 5 – 9 June 2006, LNEC.

This paper discusses the finite element development of a numerical model of 3D elements for Cabril dam, based on the main fundamental parameters of the dynamic response of the dam, obtained on several experimental results on ambient vibration tests campaigns. These experimental results are used to calibrate the numerical model of 3D finite elements considering two hypothesis to simulate the hydrodynamic water pressure: i) first assuming that the reservoir is properly simulated through associated water masses, in accordance with Westergaard's formula, and ii) second considering water finite elements.

CARACTERIZAÇÃO EXPERIMENTAL DO COMPORTAMENTO DINÂMICO DE BARRAGENS DE BETÃO COM BASE NA SUA MONITORIZAÇÃO EM CONTÍNUO

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Actualmente muitos dos sistemas de observação das grandes barragens portuguesas estão em fase de revisão e modernização, numa perspectiva de adaptação às crescentes exigências de segurança e de optimização de recursos. Neste sentido a tendência actual é para a instalação de sistemas de Recolha Automática de Dados (RAD) com vista à automatização de alguns procedimentos de observação, envolvendo não só a automatização da leitura das principais grandezas tradicionalmente observadas em cada obra, como também a medição em contínuo de grandezas dinâmicas (nomeadamente acelerações, ver Figura 1) que permitam caracterizar, em tempo real, o comportamento dinâmico das obras sob acções sísmicas, sob acções devidas ao funcionamento dos órgãos de descarga e de exploração ou sob acções associadas ao denominado ruído ambiente (trânsito local, condições meteorológicas, trabalhos na zona envolvente, etc.). O Departamento de Barragens de Betão e o Centro de Instrumentação Científica do LNEC, com o apoio da FCT, estão actualmente a desenvolver um sistema de monitorização em contínuo do comportamento dinâmico de barragens, estando prevista a instalação de um primeiro protótipo na barragem do Cabril, durante o próximo ano. Neste trabalho apresentam-se alguns resultados de ensaios de vibração ambiente efectuados na barragem do Cabril com vista à obtenção de elementos experimentais para fundamentar as decisões de projecto do futuro sistema de monitorização dinâmica, discutem-se sumariamente as vantagens deste novo tipo de sistemas, e apresentam-se as principais características do sistema que se pretende instalar pioneiramente na barragem do Cabril.

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PALEOMAGNETIC STUDY OF THE GREAT FOUM ZGUID DYKE (SOUTHERN MOROCCO): A POSITIVE CONTACT TEST RELATED TO METASOMATIC PROCESSES

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When a paleomagnetic pole is sought for in an igneous body, the host rocks should be subjected to a contact test to assure that the determined paleopole has the age of the intrusion. If the contact test is positive, it precludes the possibility that the measured magnetization is a later effect. Therefore, we investigated the variations of the remanent magnetization along cross-sections of rocks hosting the Foum Zguid dyke (Southern Morocco) and the dyke itself. A positive contact test was obtained, but it is mainly related with Chemical/Crystalline Remanent Magnetization due to metasomatic processes in the host-rocks during magma intrusion and cooling, and not only with Thermo-Remanent Magnetization as ordinarily assumed in standard studies. Paleomagnetic data obtained within the dyke then reflect the Earth magnetic field during emplacement of this well-dated (196.9±1.8 Ma) intrusion.

VARIATION OF MAGNETIC PROPERTIES IN SEDIMENTARY ROCKS HOSTING THE FOUM ZGUID DYKE (SOUTHERN MOROCCO): COMBINED EFFECTS OF RE-CRYSTALLIZATION AND FE-METASOMATISM

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The effects of dyke intrusion on the magnetic properties of host sedimentary rocks is still poorly understood. Therefore, we have evaluated bulk magnetic parameters of standard palaeomagnetic samples collected along several sections across the sediments hosting the Foum-Zguid dyke in South Morocco. The study has been completed with the evaluation of the magnetic fabric after laboratory application of sequential heating experiments. The present study shows that: (1) close to Foum Zguid dykes, the variations of the bulk magnetic parameters and of the magnetic fabric is strongly related with re-crystallization and Fe-metasomatism intensity. (2) The thermal experiments on AMS of samples collected farther from the dyke and, thus, less affected by heating during dyke emplacement, indicate that 300 – 400ºC is the minimum experimental temperature necessary to trigger appreciable transformations of the pre-existing magnetic fabrics. For temperatures higher than ca. 580ºC, the magnetic fabric transformations are fully realized, with complete transposition of the initial fabric to a fabric similar to that of samples collected close to the dyke. Therefore, measured variations of the magnetic fabric can be used to evaluate re-crystallization temperatures experienced by the host sedimentary rock during dyke emplacement. The distinct magnetic behaviour observed along the cross-sections strongly suggests that samples collected farther from the dyke margins did not experience thermal episodes with temperatures higher than 300ºC after dyke emplacement. (3) AMS data shows a gradual variation of the magnetic fabric with distance from the dyke margin, from sub-horizontal K3 away from the dyke to vertical K3 close to the dyke. Experimental heating shows that heat alone can be responsible for this strong variation. Therefore, such orientation changes should not be unequivocally interpreted as the result of a stress field (resulting from the emplacement of the dyke, for instance). (4) Magnetic studies prove to be a very sensitive tool to assess rock magnetic transformations, thermally and chemically induced by dyke intrusion in hosting sediments.

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PALEOMAGNETIC STUDY OF THE MESSEJANA PLASENCIA DYKE (PORTUGAL AND SPAIN): A LOWER JURASSIC PALEOPOLE FOR THE IBERIAN PLATE

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The only Iberian lower Jurassic paleomagnetic pole come from the "Central Atlantic Magmatic Province"-related Messejana Plasencia dyke, but the age and origin of its remanence have been a matter of discussion. With the aim of solving this uncertainty, and to go further into a better understanding of its emplacement and other possible tectonic features, a systematic paleomagnetic investigation of 40 sites (625 specimens) distributed all along the 530 km of the Messejana Plasencia dyke has been carried out. Rock magnetic experiments indicate PSD low Ti-titanomagnetite and magnetite as the minerals carrying the NRM. The samples were mostly thermally demagnetized. Most sites exhibit a characteristic remanent component of normal polarity with the exception of two sites, where samples with reversed polarities have been observed. The paleomagnetic pole derived from a total of 35 valid sites is representative of the whole structure of the dyke, and statistically well defined, with values of PLa=70.4°N, PLo=237.6°E, K=47.9 and A95=3.5°. Paleomagnetic data indicates that: (i) there is no evidence of a Cretaceous remagnetization in the dyke, as it was suggested; (ii) most of the dyke had a brief emplacement time; furthermore, two dyke intrusion events separated in time from it by at least 10,000 y have been detected; (iii) the high grouping of the VGPs directions suggests no important tectonic perturbations of the whole structure of the dyke since its intrusion time; (iv) the pole derived from this study is a good quality lower Jurassic paleopole for the Iberian plate; and (v) the Messejana Plasencia dyke paleopole for the Iberian plate is also in agreement with quality-selected European and North American lower Jurassic paleopoles and the magnetic anomalies data sets that are available for rotate them to Iberia.

THERMAL, MECHANICAL AND CHEMICAL ALTERATIONS PROMOTED ON SEDIMENTARY ROCKS HOSTING DYKE BODIES

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This work is focused on flow and propagation of magma along thick Jurassic dykes and the effects of such intrusive processes on the magnetic properties of host sedimentary rocks, which are still poorly understood. Therefore, an exhaustive study of rock magnetic and petrography analyses were performed on dolerite rocks collected along several sections across the Foum Zguid (FZD - Southern Morocco) and Messejana-Plasencia (MPD - Iberia) dykes, complemented with several sections across the sediments hosting the FZD. The study has been completed with the evaluation of the magnetic fabric carried by these sedimentary rocks after laboratory application of sequential heating experiments.

The present study shows that: i) magnetic analyses of dolerite rocks are sensitive to low to moderate metasomatic processes and cooling rate underwent by ferromagnetic minerals; ii) intrusive processes at both dykes occurred for a brief period; iii) oblique magma flow regime, rising from SW to NE, is inferred for FZD; iv) sub-vertical magma flow episodes, without discarding some sub-horizontal magma flow regimes are inferred for MPD; v) variations of the bulk magnetic parameters and of the magnetic fabric observed for sedimentary rocks hosting FZD is strongly related with re-crystallization and Fe-metasomatism intensity, with newly formed hematite as the main product; vi) the magnetic fabric obtained for sedimentary samples near the contacts with FZD was acquired during the intrusion, and could reflect either flattening in the host rock due to the stress field induced during the intrusion or the materialization of microfractures; vii) the strong compression promoted during magma emplacement leads to bulk rotations for domains nearest the contact; viii) thermal experiments of AMS on sedimentary samples collected farther from the dyke and, thus, less affected by heating, indicate that 300 – 400ºC is the minimum temperature needed to trigger appreciable transformations of the previous magnetic fabrics. Therefore, such changes in orientation should not be unequivocally interpreted as the result of a stress field.

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The present study shows that: i) magnetic analyses of dolerite rocks are sensitive to low to moderate metasomatic processes and cooling rate underwent by ferromagnetic minerals; ii) intrusive processes at both dykes occurred for a brief period; iii) oblique magma flow regime, rising from SW to NE, is inferred for FZD; iv) sub-vertical magma flow episodes, without discarding some sub-horizontal magma flow regimes are inferred for MPD; v) variations of the bulk magnetic parameters and of the magnetic fabric observed for sedimentary rocks hosting FZD is strongly related with re-crystallization and Fe-metasomatism intensity, with newly formed hematite as the main product; vi) the magnetic fabric obtained for sedimentary samples near the contacts with FZD was acquired during the intrusion, and could reflect either flattening in the host rock due to the stress field induced during the intrusion or the materialization of microfractures; vii) the strong compression promoted during magma emplacement leads to bulk rotations for domains nearest the contact; viii) thermal experiments of AMS on sedimentary samples collected farther from the dyke and, thus, less affected by heating, indicate that 300 – 400ºC is the minimum temperature needed to trigger appreciable transformations of the previous magnetic fabrics. Therefore, such changes in orientation should not be unequivocally interpreted as the result of a stress field.

FORMAÇÃO PARA UMA CULTURA DA QUALIDADE NA ENGENHARIA CIVIL

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O cenário geral empresarial português não é o ideal para poder responder aos desafios da competitividade. Tão pouco o cenário específico da gestão na engenharia civil: é exemplar pela negativa. Estas carências de gestão não se sentem nas grandes empresas, que são iguais às melhores internacionais, e sim nas médias, pequenas e micro empresas. E o problema da gestão tem a ver com a liderança e com a formação: os quadros aprendem gestão...gerindo, isto é, tentativa e erro.

Estudos efectuados na área do comportamento organizacional ensinam que, ao agir sobre o ambiente e não sobre as pessoas, se conseguem alterações mais profundas e sustentáveis: a mudança no ambiente "puxa" pelas pessoas. Não há nada mais potente para formar as pessoas do que a própria organização do trabalho combinada com a formação formal.

Investigação relativamente recente demonstrou que o português, no seio da OCDE é o que mais se motiva para atingir objectivos e resultados.

Infelizmente, a esmagadora maioria dos quadros dirigentes de todas as áreas, enfim, da elite do nosso País, não sabe soltar esse potencial; não sabe o que significa proactividade, concepção, planeamento e controlo, definição e perseguição de objectivos, gestão de uma equipa e de um projecto.

Uma das mais eficazes formas de alterar/melhorar o ambiente numa organização é introduzir o processo de certificação. Com a certificação de acordo com as Normas ISO 9000, o País poderia mobilizar-se em torno de um objectivo que funcionaria como locomotiva do nosso desenvolvimento. A China já percebeu isso: é hoje o País com mais certificados emitidos em todo o mundo.

Uma empresa certificada cria riqueza, paga impostos, cumpre a legislação de segurança, é mais exigente com os seus fornecedores (o que provoca, a montante, uma espiral de exigência), tem colaboradores mais motivados, não usa mão-de-obra ilegal, faz mais I & D, trabalha a melhoria contínua ao expor-se às auditorias e ao dar-lhes seguimento.

Como conseguir que as empresas se especializem em qualidade, quando temos baixos níveis de formação em gestão para os dirigentes e quadros intermédios e muito baixos níveis de instrução para os executantes? Como conseguir que as empresas percebam que têm de investir na formação, na ligação ao ensino superior, na investigação, e se sintam estimuladas a fazer "crescer" os colaboradores?
Nesta Comunicação apresentaram-se alguns contributos agrupados em cinco propostas de actuação, para a resposta a estas questões.

O ENSINO DA QUALIDADE NA ENGENHARIA

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Publicado em:
Actas do 2º Congresso Nacional da Construção – Construção 2004 (FEUP), Porto, Portugal, 13-15 Dezembro 2004.

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?

EXPANSÃO EM SÉRIE DE TAYLOR

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Nota: O artigo foi submetido a revisão, tendo sido aceite pelo referee, sem quaisquer alterações, em 3 de Março de 2007, para publicação.

A série de Taylor é usada em inúmeros problemas; a sua demonstração é habitualmente feita em cursos elementares de Análise, usando artifícios.

Propomos uma abordagem baseada no lema de Rolle, teorema de Lagrange e, depois de estabelecer a expressão

$$f(x)=\sum_{k=0}^{n}\prod_{i=0}^{k-1}(\xi_i-a)f^{(k)}(a)+f^{(n+1)}(\xi_{n+1})\prod_{i=0}^{n+1}(\xi_i-a),$$

onde posteriormente modelamos estes pontos com um modelo hierárquico, $\xi_o=x$, e $\xi_i|_{\xi_{i-1}}$ é uma variável aleatória simétrica no seu suporte (a,ξ_{i-1}), um modelo intuitivo quando se pretende um resultado válido para qualquer função $f \in C^{n+1}$. Usando valores esperados condicionais, obtém-se de imediato o resultado tradicional.
Esta abordagem é, também, uma forma de ilustrar a extensão do teorema sobre a obtenção do valor médio da variável Y como valor médio da variável E[Y | X], quando é dado um modelo hierárquico em mais do que dois passos, uma questão raramente exemplificada de forma que não seja artificiosa.
Com modelos mais gerais é possível obter expressões diversas para o resto R(x), por exemplo a de Schlömilch.

DATA PROCESSING FOR SAFETY CONTROL OF BRIDGES IN REAL TIME

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The observation of structure's behaviour, especially long-term observation, has had a large improvement due to the introduction of new techniques for automatic acquisition of the measurements. Automatic acquisition gives us the possibility of reading several equipments continuously, simultaneously, without the presence of operators, plus the capability of establishing a remote connection to a centre of studies through phone, radio, GSM or Internet.

In order to take advantage of automatic acquisition and from the new developments that provided not only the improvement of existent sensors based on the recent technologies, but also the upgrading of storage and acquisition equipment, it became necessary the development of new methodologies for data processing.

For the data management and analysis, we need to have reliable measurements from each sensor and information of the relations between different sensors and the evolution of the data in time.

Some of this information is now possible to get directly from the dataloggers with the definition of sub routines that introduced on the acquisition program. This way they are done immediately after the readings, and we have the possibly of repeating some measurements if we detect any anomalous data. These procedures include validation of signals, measurements and tendencies.

On the other hand, to guarantee the observation of the structure in real time, alert and alarm levels have to be established to control, permanently and in situ, the development of selected variables, allowing a more efficient evaluation of the conditions of safety of the structure.

This paper will describe the developed methodologies for data processing of bridge monitoring data, in real time.

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DEVELOPMENT OF DAM FINITE ELEMENT MODELS FOR DYNAMIC ANALYSIS USING AMBIENT VIBRATION TEST RESULTS

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Publicado em:
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This paper discusses the finite element development of a numerical model of 3D elements for Cabril dam, based on the main fundamental parameters of the dynamic response of the dam, obtained on several experimental results on ambient vibration tests campaigns. These experimental results are used to calibrate the numerical model of 3D finite elements considering two hypothesis to simulate the hydrodynamic water pressure: i) first assuming that the reservoir is properly simulated through associated water masses, in accordance with Westergaard's formula, and ii) second considering water finite elements.

CARACTERIZAÇÃO EXPERIMENTAL DO COMPORTAMENTO DINÂMICO DE BARRAGENS DE BETÃO COM BASE NA SUA MONITORIZAÇÃO EM CONTÍNUO

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Actualmente muitos dos sistemas de observação das grandes barragens portuguesas estão em fase de revisão e modernização, numa perspectiva de adaptação às crescentes exigências de segurança e de optimização de recursos. Neste sentido a tendência actual é para a instalação de sistemas de Recolha Automática de Dados (RAD) com vista à automatização de alguns procedimentos de observação, envolvendo não só a automatização da leitura das principais grandezas tradicionalmente observadas em cada obra, como também a medição em contínuo de grandezas dinâmicas (nomeadamente acelerações, ver Figura 1) que permitam caracterizar, em tempo real, o comportamento dinâmico das obras sob acções sísmicas, sob acções devidas ao funcionamento dos órgãos de descarga e de exploração ou sob acções associadas ao denominado ruído ambiente (trânsito local, condições meteorológicas, trabalhos na zona envolvente, etc.). O Departamento de Barragens de Betão e o Centro de Instrumentação Científica do LNEC, com o apoio da FCT, estão actualmente a desenvolver um sistema de monitorização em contínuo do comportamento dinâmico de barragens, estando prevista a instalação de um primeiro protótipo na barragem do Cabril, durante o próximo ano. Neste trabalho apresentam-se alguns resultados de ensaios de vibração ambiente efectuados na barragem do Cabril com vista à obtenção de elementos experimentais para fundamentar as decisões de projecto do futuro sistema de monitorização dinâmica, discutem-se sumariamente as vantagens deste novo tipo de sistemas, e apresentam-se as principais características do sistema que se pretende instalar pioneiramente na barragem do Cabril.

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MODELOS NUMÉRICOS PARA ANÁLISE DO COMPORTAMENTO DE BARRAGENS DE BETÃO. SIMULAÇÃO DE ROTURAS COM BASE EM FORMULAÇÕES DE DANO

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Provas Concluídas em: 22 de Junho de 2006

A modelação numérica da fissuração em grandes estruturas de betão, como é o caso das barragens abóbada, pode ser efectuada, em muitas situações, com base na hipótese de fissuração distribuída, utilizando leis constitutivas de dano contínuo com enfraquecimento para descrever a rotura por tracção.
A consideração do enfraquecimento à tracção, dependente do valor da energia de fractura do material, conduz à ocorrência de fenómenos de localização da rotura e exige a adopção de alguns cuidados ao nível da modelação numérica quando se utiliza o Método dos Elementos Finitos. Nomeadamente, há que adoptar formulações que permitam garantir que a energia dissipada no processo de rotura é independente da discretização adoptada, ou seja, que permitam assegurar a objectividade das soluções numéricas.
Utilizando uma formulação de elementos finitos tridimensionais e uma lei constitutiva de dano isotrópico com duas variáveis de dano independentes, concebida para simular o efeito de enfraquecimento em tracção e em compressão de forma separada, apresentam-se neste trabalho resultados numéricos relativos à análise do comportamento da barragem do Cabril para cenários correntes e de rotura. Adoptam-se discretizações em elementos finitos com diferentes níveis de refinamento, com vista a analisar a objectividade das soluções numéricas, utilizando uma formulação consistente para calcular os valores aparentes da energia específica de fractura, mais adequados a cada discretização.

DOMAIN DECOMPOSITION METHODS FOR NON-NEWTONIAN FLUIDS

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Doutoramento em: Matemática
Grau Concedido por: IST – Universidade Técnica de Lisboa
Orientadores: Adélia Sequeira e Nadir Arada
Provas Concluídas em: 22 de Dezembro de 2006

O objectivo desta tese é o estudo da implementação numérica de um método de decomposição de domínios com precondicionamento aplicado à aproximação por elementos finitos de escoamentos estacionários de fluidos não-Newtonianos viscoelásticos de Oldroyd-B. As equações constitutivas deste modelo conduzem a um sistema não linear misto de equações com derivadas parciais que, através de um argumento de ponto fixo, é possível desacoplar num sistema de equações de Navier-Stokes e numa equação de transporte tensorial. Aplica-se um algoritmo de Schwarz modificado a cada um dos problemas anteriores que envolve precondicionadores por blocos para o sistema de Navier-Stokes. Para a validação do método de decomposição de domínios com precondicionamento consideram-se dois problemas teste, os escoamentos na contracção abrupta 4:1 e na cavidade bidimensional. O método é ainda aplicado a um canal com bifurcação e analisam-se os resultados numéricos correspondentes.

THE USE OF ROCK MAGNETIC METHODS TO STUDY THERMAL AND MECHANICAL PROCESSES. SALDANHA MASSIF, AND FOUM ZGUID AND MESSEJANA-PLASENCIA DYKES

Carvalho da Silva, Pedro Manuel Fernandes

Doutoramento em: Física (Geofísica Interna)
Grau Concedido por: Universidade de Lisboa
Orientadores: Jorge Miguel de Alberto Miranda e Fernando Ornelas Marques
Provas Concluídas em: 20 de Dezembro de 2006

Publicado em:
Revista Recursos Humanos Magazine no nº de Janeiro/Fevereiro 2003

The present thesis focuses on the study of magnetic properties of rocks from two distinct geological settings: i) The Mid-Atlantic Ridge (MAR) – case study of Saldanha Massif (Part I) and ii) Central Atlantic Magmatic Province (CAMP) – case studies of Messejana-Plasencia dyke (Iberian Peninsula) and Foum Zguid dyke (Southern Morocco) in continental crust (Part II). For Part I, the causes of temporal and spatial variability of Natural Remanent Magnetisation (NRM) along Saldanha Massif were investigated for posterior correlation with the geological framework and distance to the ridge axis. Therefore, a group of 30 basalt blocks were submitted to rock magnetism studies. The results show that: i) titanomagnetite (TM) appears to be the original magnetic phase; ii) titanomaghemite appears as a low-temperature oxidation product of primary TM; iii) variations of NRM intensity inside the study area are controlled by the grain size and oxidation state; v) Single-domain TM grains show an inverse linear relationship between NRM intensity and oxidation degree; vi) the higher oxidation degrees are presented by samples located within Saldanha Massif limits. Detachment fault surfaces that can promote preferred pathways for fluid circulation in an essentially shallow environment thus explaining the higher low-temperature oxidation degrees of the Massif samples, is the hypothesis proposed; and vii) samples outside Saldanha Massif limits show an increase in the oxidation degree with distance from the FAMOUS spreading axis. In Part II, the main objectives were focused on flow and propagation of magma along thick Jurassic dykes and the effects of such intrusive processes on the magnetic properties of host sedimentary rocks, which are still poorly understood. Therefore, an exhaustive study of rock magnetic and petrography analyses was performed on dolerite rocks collected along several sections across the Foum Zguid (FZD - Southern Morocco) and Messejana-Plasencia (MPD - Iberia) dykes, complemented with several sections across the sediments hosting the FZD. The study has been completed with the evaluation of the magnetic fabric carried by these sedimentary rocks after laboratory application of sequential heating experiments. The present study shows that: i) magnetic analyses of

dolerite rocks are sensitive to low to moderate metasomatic processes and cooling rate underwent by ferromagnetic minerals; ii) intrusive processes at both dykes occurred for a brief period; iii) oblique magma flow regime, rising from SW to NE, is inferred for FZD. Such result agrees with the spatial location and orientation of this dyke relative to the core of the CAMP; iv) sub-vertical magma flow episodes, without discarding some sub-horizontal magma flow regimes are inferred for MPD; v) variations of the bulk magnetic parameters and of the magnetic fabric observed for sedimentary rocks hosting FZD is strongly related with re-crystallization and Fe-metasomatism intensity, with newly formed hematite as the main product; vi) the magnetic fabric obtained for sedimentary samples near the contacts with FZD was acquired during the intrusion, and could reflect either flattening in the host rock due to the stress field induced during the intrusion or the materialization of microfractures; vii) the strong compression promoted during magma emplacement leads to bulk rotations for domains nearest the contact; viii) thermal experiments of AMS on sedimentary samples collected farther from the dyke and, thus, less affected by heating, indicate that 300 – 400ºC is the minimum temperature needed to trigger appreciable transformations of the previous magnetic fabrics. Therefore, such changes in orientation should not be unequivocally interpreted as the result of a stress field; ix) the VGP achieved for FZD igneous rocks corresponds to (E) = 250.7º, l(N) = 67.0º, with K = 281 and A95 = 3.4º; and x) a similar movement between Iberian Peninsula and North Africa for the last ~200 Ma is proposed.


02

ENGENHARIA DE ELECTRÓNICA DE TELECOMUNICAÇÕES E DE COMPUTADORES

Anuário Científico 2006

ISEL

INFORMATION THEORETIC TEXT CLASSIFICATION USING THE ZIV-MERHAV METHOD

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Most approaches to text classification rely on some measure of (dis)similarity between sequences of symbols. Information theoretic measures have the advantage of making very few assumptions on the models which are considered to have generated the sequences, and have been the focus of recent interest. This paper addresses the use of the Ziv-Merhav method (ZMM) for the estimation of relative entropy (or Kullback-Leibler divergence) from sequences of symbols as a tool for text classification. We describe an implementation of the ZMM based on a modified version of the Lempel-Ziv algorithm (LZ77). Assessing the accuracy of the ZMM on synthetic Markov sequences shows that it yields good estimates of the Kullback-Leibler divergence. Finally, we apply the method in a text classification problem (more specifically, authorship attribution) outperforming a previously proposed (also information theoretic) method.

Publicado em:
Lecture Notes in Computer Science, Springer, Volume 3523/2005, June 7-9, 2005, Pages 355-362 IbPRIA 2005 - 2nd Iberian Conference on Pattern Recognition and Image Analysis

CO-SYNTHESIS OF A CONFIGURABLE SOC PLATFORM BASED ON A NETWORK ON CHIP ARCHITECTURE

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Publicado em:
ASP-DAC, 2006 - 12th Asia and South Pacific Design Automation Conference, January 2006.

The constant increase of gate capacity and performance of configurable hardware chips made it possible to implement systems-on-chip (SoC) able to tackle the demanding requirements of many embedded systems. In this paper, we propose an approach to the design space exploration of a configurable SoC (CSoC) platform based on a network on chip (NoC) architecture for the execution of dataflow dominated embedded systems. The approach has been validated with the design of a color image compression algorithm in an FPGA.

AREA/PERFORMANCE IMPROVEMENT OF NOC ARCHITECTURES

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The design of electronic systems in a System-on-Chip (SoC) depends on the reliable and efficient interconnection of many different components. The Network-on-Chip (NoC) has emerged as a scalable communication infrastructure with high bandwidth able to tackle the communication needs of future SoC. In this paper, we present a configurable router that can be tailored to the specific bandwidth needs of the system in order to reduce the area overhead associated with the NoC.

Publicado em:
Lecture Notes in Computer Science, vol. 3985, Springer, ISBN: 3-540-36708-X 2nd ARC 2006 - 2th International Workshop on Applied Reconfigurable Computing, March 2006.

HYBRID GENERATIVE/ DISCRIMINATIVE TRAINING OF RADIAL BASIS FUNCTION NETWORKS

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Publicado em:
European Symposium on Neural Networks (ESANN 2006), Bruges, Bélgica, Abril 2006

We propose a new training algorithm for radial basis function networks (RBFN), which incorporates both generative (mixture-based) and discriminative (logistic) criteria. Our algorithm incorporates steps from the classical expectation-maximization algorithm for mixtures of Gaussians with a logistic regression step to update (in a discriminative way) the output weights. We also describe an incremental version of the algorithm, which is robust regarding initial conditions. Comparison of our approach with existing training algorithms, on (both synthetic and real) binary classification problems, shows that it achieves better performance.

LIGHT FILTERING PROPERTIES IN A-SIC:H MULTILAYER STRUCTURES: A SPICE MODEL

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A SPICE model of a-SiC:H/ a-Si:H pin/pin detector with voltage controlled spectral sensitivity is presented. The equivalent electric circuit able to describe the behavior of the multilayer structure under non-uniform illumination is composed of two series connected diodes, representing the pin structures, with two nonlinear current sources in parallel, representing the photogeneration for different steady state RGB illumination, with their value depending also on the thickness of the absorber layer and the built-in potential of the diodes. This device represents the 1D model of the LSP (Laser Scanned Photodiode) and may be interconnected in a 2D array trough resistors, modeling the high resistivity of the a-SiC:H layers. Electrical simulations were performed for different transducer configurations and illumination conditions and compared with the experimental data. The influence of the lateral and transverse resistors and built-in potential of the diodes on sensor parameters like spatial resolution, and signal amplitude are analyzed. A physical model supported by the electrical simulation gives insight into the methodology used for image representation and color discrimination.

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2006 Spring Proceedings Microelectronic Device Processing and Fabrication - Symposium A Amorphous and Polycrystalline Thin-Film Silicon Science and Technology — 2006 MRS Proceedings Volume 910

BAND GAP ENGINEERING AND ELECTRICAL FIELD TAILORING FOR VOLTAGE CONTROLLED SPECTRAL SENSITIVITY

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2006 Spring Proceedings Microelectronic Device Processing and Fabrication - Symposium A Amorphous and Polycrystalline Thin-Film Silicon Science and Technology — 2006 MRS Proceedings Volume 910

Stacked ITO/(a-SiC:H)pinpi /(a-Si:H)i'n/ITO color sensitive detectors are analyzed using the laser scanned photodiode technique. Results show that band gap engineering together with the laser scanned photodiode technique allows a voltage controlled shift of the collection regions, allowing color discrimination at readout voltage that cancels the self-bias effect induced by the steady state illumination, across the back diode. The threshold voltage between green and red discrimination depends on the thickness ratio between a-Si:H (-i?)/a-SiCH (-i) layers. As this ratio increases the self-reverse effect due to the front absorption will be balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias. The various design parameters and the optical readout process trade-offs are discussed and supported by a 2D numerical simulation. A self-bias model is proposed to explain the voltage controlled spectral sensitivity.

MODELING CORRELATION NOISE STATISTICS AT DECODER FOR PIXEL BASED WYNER-ZIV VIDEO CODING

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Distributed video coding (DVC) is a new video coding paradigm based on two key Information Theory results: the Slepian-Wolf and Wyner-Ziv theorems. Recently, promising results were shown in Wyner-Ziv (WZ) video coding, a particular case of DVC. In the literature, many practical WZ coding approaches model the correlation noise between the original frame and the so-called side information by a given distribution whose relevant parameters are estimated offline, at the encoder. This paper proposes an algorithm to estimate, at the decoder, and at the frame level, the correlation or error distribution between the original and the side information frames, in a way which is as efficient as the estimation made at the encoder based on the original information. This approach relieves the encoder from the task to perform this estimation based on the original information, which is rather important since DVC solutions are typically adopted under low encoder complexity constraints.

Publicado em:
Picture Coding Symposium, Beijing, China, April 2006

SAR MOVING TARGETS PROCESSING FOR SMALL AIRBORNE PLATFORMS

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This paper presents a methodology to retrieve the full velocity vector of moving targets inducing Doppler-shifts beyond the Nyquist limit determined by the pulse repetition frequency (PRF). The proposed approach exploits the linear dependence (not subject to PRF limitations) of the Doppler-shift with respect to the slant-range velocity, at each wavelength. By combining the developed scheme to retrieve the slant-range velocity with a methodology proposed earlier to estimate the velocity vector magnitude, the full velocity vector is unambiguously retrieved. The proposed approach is very efficient from the computational point of view and uses data from a single channel SAR channel, being therefore adequate for use in low resources platforms such as UAVs.

Publicado em:
6th European Conference on Synthetic Aperture Radar, 16-18 May 2006, Dresden, Germany, Pages 384-387

02

CONCEPTS OF SIMULTANEOUS USE IN MOBILE AND WIRELESS COMMUNICATIONS

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Wireless communication research is evolving towards integration, inter-working and convergence of wireless systems, which will lead to several concepts of simultaneous use. In the present paper, a coherent set of 10 concepts of simultaneous use is identified, and structured into a space of simultaneous use, where services, systems and operators act as building components. A high level analysis is performed, where the pros and cons of the different concepts are identified. Illustrative examples are also provided for some concepts. Several parameters are listed for the evaluation of simultaneous use concepts (e.g., cost, throughput and complexity), depending on taking a users' or an operators' perspective. One of the largest benefits of this systematic identification of simultaneous use concepts is the identification, from the perspective of users and operators, of essential R&D issues on inter-working and integration, which will lead to a promising pervasive wireless communications future.

Publicado em:
Special Issue on Elective Topics towards Vision to Reality of the Wireless Future, Wireless Personal Communications, Springer,Vol. 37, No 3, May 2006, pp. 317-328

AN ADVISER FOR EFFICIENTLY RESOLVE EMAIL FEATURE INTERACTIONS

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Publicado em:
Proceedings of "International Conference on Internet and Web Applications and Services", ICIW'06, IEEE Computer Society

Internet applications, such as Email, VoIP and WWW, have been enhanced with many features. However, the introduction and modification of features may result in undesired behaviors, and this effect is known as feature interaction-FI.

We describe a distributed FI resolution, based on advisers. The adviser follows deontic rules and is implemented with Java technology. In case of failure of one Internet node, message processing is not compromised.

Our proposal was customized and tested to James Email server, and the results satisfy main requirements and do not compromise performance.

PARAMETERS FOR THE DEFINITION OF SCENARIOS FOR CRRM PERFORMANCE EVALUATION

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This paper addresses the RRM and CRRM reference scenarios state of the art. Many researchers use simulation tools for their work, using different approaches and scenarios, disabling the possibility to evaluate and compare results among them. Thus, this paper besides pointing out the different activities on reference scenarios, proposes a set of scenarios for RRM and CRRM for GERAN, UTRAN and WLAN. This paper constitutes a first approach of identification of key para-meters related with RRM/CRRM performance evaluation.

Publicado em:
13th IEEE Mediterranean Electrotechnical Conference, Málaga, Espanha, Maio, 2006

02

KALMAN FILTERING FOR ACQUISITION OF GNSS SIGNALS IN HIGHLY-MANOEUVRABLE RECEIVERS

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GNSS receivers in highly-manoeuvrable platforms, such as military aircraft and rockets, bear large values of acceleration which prevents the use of simple signal acquisition techniques. Herein, we propose a new approach to the acquisition problem which is divided into two parts: a coarse code delay/Doppler frequency acquisition algorithm followed by a refinement (and validation) algorithm based on two banks of Kalman filters. The first bank allows to obtain estimates of the code delay and the Doppler frequency. The second bank permits to refine the frequency estimates.

Publicado em:
Proceedings of the IEEE/ION Position Location and Navigation Symposium, PLANS2006, May 23-27, 2006, San Diego, CA, USA.

02

STROBE PULSE DESIGN FOR MULTIPATH MITIGATION IN BOC GNSS RECEIVERS

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

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Proceedings of the IEEE/ION Position Location and Navigation Symposium, PLANS2006, May 23-27, 2006, San Diego, CA, USA.

IMPROVING TRANSFORM DOMAIN WYNER-ZIV VIDEO CODING PERFORMANCE

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Publicado em:
IEEE International Conference on Acoustics, Speech and Signal Processing, Toulouse, France, May 2006

Distributed video coding (DVC) is a new video coding paradigm based on two key Information Theory results: the Slepian-Wolf and Wyner-Ziv theorems. A particular case of DVC, the so-called Wyner-Ziv coding, deals with lossy source coding with side information at the decoder and enables a flexible allocation of complexity between the encoder and the decoder. This paper proposes an improved transform domain Wyner-Ziv video codec including: 1) the integer block-based transform defined in the H.264/MPEG-4 AVC standard, 2) a quantizer with a symmetrical interval around zero for AC coefficients, and a quantization step size adjusted to the transform coefficient bands dynamic range, and finally and 3) advanced frame interpolation for side information generation. The combination of these tools brings significant rate-distortion (RD) gains regarding the state-of-the-art results available in the literature.

ADAPTIVE METHOD IN SPACE FOR THE RESOLUTION OF MAXWELL'S EQUATIONS

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In this paper a scheme to obtain an adaptive method in space for the resolution of Maxwell's equations is presented. Using interpolating wavelets it is possible to obtain an adaptive grid allowing a reduction of the computation time and an economy of the computational resources. Using the staggered grid model the dispersion proprieties are improved with the increase of the interpolating polynomial, despite of a more restricted stability factor.

Publicado em:
ICT2006 – 13th International Conference on Telecommunications, Funchal, Madeira, 9-12 Maio 2006

ADMISSION REGULATION OF TRAFFIC TO IMPROVE PUBLIC TRANSPORT IN URBAN AREAS

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We correlate rate of entering traffic in Lisbon, Portugal, and the speed of buses. The admission rate was reduced by varying green and red light times at one entry point of the city, permitting buses on some routes to maintain constant average speed during rush hour, rather than dropping.

Publicado em:
Transportation Science and Logistics Society Urban Transportation Planning Models Special Interest Group, USA, May 2006

02

UBIQUITOUS KNOWLEDGE MODELING FOR DIALOGUE SYSTEMS

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The main general problem that we want to address is the reconfiguration of dialogue systems to work with a generic plug-and-play device. This paper describes our research in designing knowledge--based everyday devices that can be dynamically adapted to spoken dialogue systems. We propose a model for ubiquitous knowledge re-presentation that enables the spoken dialogue system to be aware of the devices belonging to the domain and of the tasks they provide. We consider that each device can be augmented with computational capabilities in order to support its own knowledge model. A knowledge--based broker adapts the spoken dialogue system to deal with an arbitrary set of devices. The knowledge integration process between the knowledge models of the devices and the knowledge model of the broker is depicted. This process was tested in the home environment domain.

Publicado em:
Proceedings of the 8th International Conference on Enterprise Information Systems (ICEIS 2006), Maio 2006, Pages 143-150

ENHANCING A PERVASIVE COMPUTING ENVIRONMENT WITH LEXICAL KNOWLEDGE

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Publicado em:
Proceedings of the 2nd International Conference on Knowledge Engineering and Decision Support (ICKEDS 2006), Maio 2006, Pages 307-312

A pervasive computing environment consists typically of a large heterogeneous collection of networked devices. This paper describes the use of lexical knowledge to improve a pervasive computing environment. In an ongoing research project, we are exploring ways to enable non-technical users to manage and control their home environment that is particularly hostile. We assume that each device belonging to the pervasive environment has its own knowledge model, linked to lexical resources, with the purpose of defining a semantic interface. This approach tries to reach the pervasive essence of the natural language. The coverage of handmade lexical resources is limited, coverage problems remain for applications involving specific domains or involving multiple languages. Our recent efforts are directed towards the technology development, focusing on devices that are household appliances. This work is a contribution to facilitate, specially: the generation of multilingual device descriptions, the automatic build of device's graphical user interfaces, and on the fly adaptation of a spoken dialogue system to the pervasive environment.

A TASK REPOSITORY FOR AMBIENT INTELLIGENCE

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This paper describes a task repository, a device semantic interface to express device capabilities, and an advice algorithm that suggests the best task-device pair to satisfy a request. The purpose of the task repository is the adaptation of a pervasive environment (Ambient Intelligence) to support natural language applications, such as a natural language interface. The task repository has a predefined group of concepts linked to linguistic and semantic resources and is updated, at runtime, with task descriptors associated with a set of heterogeneous devices. We assume that each device, belonging to the pervasive environment, holds its own semantic interface essentially composed of task descriptors. This approach tries to reach the ubiquitous essence of natural language, because the coverage of handmade lexical resources is limited, coverage problems remain for applications involving specific domains or involving multiple languages. Furthermore, we reduce the interface device problem to a database access problem. An environment simulator with the respective set of devices is depicted.

Publicado em:
Natural Language Processing and Information Systems, Maio 2006, Pages 81-7 NLDB 2006 - The 11th International Conference on Applications of Natural Language to Information Systems

A FRAMEWORK TO INTEGRATE UBIQUITOUS KNOWLEDGE MODELING

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Publicado em:
Proceedings of the 5th International Conference on Language Resources and Evaluation (LREC 2006), Maio 2006, Pages 2361-2366

This paper describes our contribution to let end users configure mixed-initiative spoken dialogue systems to suit their personalized goals. The main problem that we want to address is the reconfiguration of spoken language dialogue systems to deal with generic plug-and-play artifacts. Such reconfiguration can be seen as a portability problem and is a critical research issue. In order to solve this problem we describe a hybrid approach to design ubiquitous domain models that allows the dialogue system to perform recognition of available tasks on the fly. Our approach considers two kinds of domain knowledge: the global knowledge and the local knowledge. The global knowledge, that is modeled using a top-down approach, is associated at design time with the dialogue system itself. The local knowledge, that is modeled using a bottom-up approach, is defined with each one of the artifacts. When an artifact is activated or deactivated, a bilateral process, supported by a broker, updates the domain knowledge considering the artifact local knowledge. We assume that everyday artifacts are augmented with computational capabilities and semantic descriptions supported by their own knowledge model. A case study focusing a microwave oven is depicted.

LOW LEAKAGE CURRENT A-SI: H/A-SIC:H N–I–P PHOTODIODE WITH CR/A-SINX FRONT CONTACT

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This paper presents the design and fabrication process of an a-Si:H/a-SiC:H heterojunction n–i–p photodiode developed for low-level light detection applications. The critical fabrication issues associated with deposition of device-quality materials, tailoring of defects at the i–p interface, film patterning, junction passivation, and contact formation are discussed. A significant reduction of the leakage current down to not, vert, similar10 pA/cm^2 at reverse bias of 1 V has been achieved by the introduction of not, vert, similar2 nm graded and not, vert, similar4 nm a-SiC:H buffer layers between the i- and p-layers. To preserve interface integrity, a semi-transparent Cr film with a-SiNx anti-reflection coating is used as a front contact. It is found that such contact induces lower leakage than transparent conductive oxide (TCO) contacts, which can cause a degradation of the p–i interface. A drawback of the semi-transparent metal contact is the optical loss, which can be minimized by thinning the metal layer and optimizing the anti-reflection coating. Quantum efficiency up to 52% is achieved for the optimized photodiode.

Publicado em:
Journal of Non-Crystalline Solids Volume 352, Issues 9-20, 15 June 2006, Pages 1837-1840

SPICE MODEL FOR A LASER SCANNED PHOTODIODE TRICOLOR IMAGE SENSOR

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

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A SPICE model of the three color a-SiC:H/a-Si:H p–i–n/p–i–n detector operation is presented. The equivalent electric circuit able to describe the behavior of the multilayer structure under non-uniform illumination is composed of two series connected diodes, representing the p–i–n structures, with two non-linear current sources in parallel, representing the photogeneration for different steady-state RGB illumination, with their values depending on the light penetration depth and intensity of the impinging light. This device represents the 1D model of the Laser Scanned Photodiode and may be interconnected in a 2D array trough resistors, modeling the high resistivity of the a-SiC:H layers. Electrical simulations were performed for different illumination conditions, and they are compared with the experimental data. The influence of the electrical model parameters on sensor characteristics is analyzed. A physical model supported by the electrical simulation gives insight into the methodology used for image representation and color discrimination.

LIGHT FILTERING IN A-SIC: H MULTILAYERS STACKED DEVICES USING THE LSP TECHNIQUE

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Light filtering in a-SiC:H stacked multilayer devices is analyzed, using the Laser Scanned Photodiode technique. Results show that the p–i–n–p–i–n device, under appropriated read-out voltages, behaves itself as an imager and a filter giving information not only on the position where the optical image is absorbed but also on its wavelength and intensity. Identification of the red, green and blue components of the spectrum and simultaneous image recognition were achieved at read-out voltages that are able to cancel the self-bias effect due to the different light penetration depth. These voltages shift from positive to negative values as the wavelength of the impinging photons across the back absorber increases. A numerical simulation supports the color filter analysis.

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THE LASER SCANNED PHOTODIODE: THEORETICAL AND ELECTRICAL MODELS OF THE IMAGE SENSOR

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The laser scanned photodiode (LSP) presents a new concept of image sensor with application in fields where low cost, large area and design simplicity are of major importance. Over the past few years this type of sensor has been under investigation and development, where several structures have been tested and characterized. In this work we present the physical explanation of device operating principle, with recourse to numerical simulation applied to structures with different compositions of the doped layers. An electrical model for this type of device is presented, enabling a fast evaluation of the device characteristics by means of an electrical simulation program.

RADIATION-INDUCED DEFECTS IN A-SI: H BY 1.5 MEV HE4 PARTICLES STUDIED BY PHOTOCONDUCTIVITY AND PHOTOTHERMAL DEFLECTION SPECTROSCOPY

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We report radiation effects on intrinsic a-Si:H thin films subjected to a 1.5 MeV He4 beam for particle fluences up to 1016 cm-2. Photothermal deflection spectroscopy is used to obtain information on the sub-gap density of states. Photoconductivity detects changes in the μτ-product of the electrons. Steady-state photocarrier grating technique is used for measuring the ambipolar diffusion length and estimating the hole μτ-product. The 1.5 MeV He4 beam radiation results in pronounced changes in the a-Si:H absorption spectrum. Optical absorption due to deep defects increases with particle fluence by more than one order of magnitude. Electronic transport properties consistently degrade with increasing particle fluence and correlate with the density of radiation-induced defects.

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ON THE USE OF INDEPENDENT COMPONENT ANALYSIS FOR IMAGE COMPRESSION

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This paper addresses the use of independent component analysis (ICA) for image compression. Our goal is to study the adequacy (for lossy transform compression) of bases learned from data using ICA. Since these bases are, in general, non-orthogonal, two methods are considered to obtain image representations: matching pursuit type algorithms and orthogonalization of the ICA bases followed by standard orthogonal projection.

Several coder architectures are evaluated and compared, using both the usual SNR and a perceptual quality measure called picture quality scale. We consider four classes of images (natural, faces, fingerprints, and synthetic) to study the generalization and adaptation abilities of the data-dependent ICA bases. In this study, we have observed that: bases learned from natural images generalize well to other classes of images; bases learned from the other specific classes show good specialization. For example, for fingerprint images, our coders perform close to the special-purpose WSQ coder developed by the FBI. For some classes, the visual quality of the images obtained with our coders is similar to that obtained with JPEG2000, which is currently the state-of-the-art coder and much more sophisticated than a simple transform coder.

We conclude that ICA provides an excellent tool for learning a coder for a specific image class, which can even be done using a single image from that class. This is an alternative to hand tailoring a coder for a given class (as was done, for example, in the WSQ for fingerprint images). Another conclusion is that a coder learned from natural images acts like an universal coder, that is, generalizes very well for a wide range of image classes.

A-SIC:H/A-SI:H TANDEM STRUCTURE ANALYSIS FOR RGB COLOR RECOGNITION IN LSP DEVICES

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A device structure based on a a-SiC:H/a-Si:H pin/pin tandem structure is proposed for a proper color separation process that takes advantage of the different light spectrum filtering properties of the a-Si:H and a-SiC:H absorbers. We have analyzed a tandem pin–pin device with the following structure deposited using the plasma enhanced chemical vapor deposition (PECVD) technique: ITO/p-type a-SiC:H (20 nm)/a-SiC:H (200 nm)/n-type a-SiC:H (20 nm)/p-type a-SiC:H (20 nm)/a-Si:H (1500 nm)/n-type a-Si:H (50 nm)/ITO. Carbon concentration in the top a-SiC:H cell produces an optical gap of about 2.0 eV. A numerical simulation of the internal electrical configuration of the device under different wavelength radiation supports our analysis of the device operation. The bias dependence of the device output is explained by taking into account, from the point of view of the color sensor applications, considerations about an asymmetric reaction of the internal electric fields to the externally imposed forward bias and a self-biasing effect of the sub-cells under certain unbalanced light generation of carriers. The simulation shows that this structure permits a good recognition of blue color under reverse bias and red color under forward bias conditions. The acquisition of a satisfactory RGB image mapping by controlling the applied bias is possible but remains problematic due to the poor separation of the green component at any value of the applied bias. A simple algorithm is proposed to deduce the green component of the light by combining the previously acquired information about the total intensity of the incident radiation and about the blue and red components.

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SPEAKER CHARACTERIZATION WITH MLSF

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IEEE Odyssey 2006 – The Speaker and Language Recognition Workshop

The work described in this paper concerns the analysis of an alternative feature for speaker characterization, in the context of speaker recognition: Line Spectrum Frequencies (LSF), but derived from mel-filter bank energies. This new feature, that we denominate mel-LSFs (MLSFs), shows similar performance comparing to MFCCs for male speakers, one of the most common feature found in speaker recognition, but for female speakers MLSFs performs better than MFCCs. When combined with mel LSFs differences, MLSFs feature overcomes the performance of the MFCCs for male and female speakers, even with temporal delta, ?MFCCs, included. Performance is measured in the context of speaker verification, using EER and minimum HTER. Detection error threshold (DET) curves are also presented, as well as HTER curves.The main objective of this study is to compare different features performances with a common framework, from what a standard support vector machine recogniser was developed. Tests are based on the cellular component of the "2002 NIST Speaker Recognition Evaluation Corpus".

REPRESENTAÇÃO DE FUNÇÕES USANDO O SPR

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O método de representação esparsa de pontos (SPR) é uma técnica de adaptabilidade especial utilizada para resolução numérica de equações diferenciais parciais evolutivas cujas soluções são suaves na maior parte do domínio mas também possuem regiões não suaves localizadas associadas a choques ou singularidades [1, 2, 3, 4]. Nessa representação são utilizados algoritmos de decomposição e reconstrução que utilizam a transformada wavelet interpolatória em multinível. Os coeficientes wavelets de tal transformada possuem valores mais significativos nas regiões onde as soluções são mais irregulares. A ideia principal desse método é representar as soluções em uma malha menos refinada uniforme acrescida de um conjunto de pontos associados as posições espaciais aonde a solução apresenta as estruturas localizadas. Esse conjunto de pontos é definido por meio da eliminação dos coeficientes wavelets menores que um certo parâmetro de truncamento a ser definido. A partir dessa representação procede-se a diferenciação dos operadores espaciais usando o método de diferenças finitas. Neste trabalho são estudadas as representações de um conjunto de soluções típicas das Equações de Maxwell e das equações de água rasa analisando-se as relações entre o grau de esparsidade, estrutura multinível da representação e o parâmetro de truncamento. Esse estudo faz parte da avaliação das estratégias de optimização e escolha das estruturas de dados do método SPR.

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Encontro Nacional da Sociedade Portuguesa de Matemática, 20 a 23 de Junho 2006, Lisboa.

AN AMORPHOUS SIC/SI IMAGE PHOTODETECTOR WITH VOLTAGE-SELECTABLE SPECTRAL RESPONSE

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The sensitive devices are multilayer stacked structures p–i–n/p–i–n based on a-SiC:H and a-Si:H between two transparent conductive contacts. The thickness and the absorption coefficient of the front p–i–n cell is optimized for blue collection and red transmittance and the thickness of the back one adjusted to achieve full absorption in the green and high collection in the red spectral ranges. Color discrimination is achieved through the modulation of one, two or both cell depletion regions by an applied external voltage.

The devices are characterized through the analysis of the photocurrent and spectral response under different steady state optical bias and applied voltages. In order to achieve full color discrimination and to evaluate the sensors responsivity to different light wavelengths, the photocurrent generated by a modulated red light is measured under different optical/electric bias. The sensor element is illuminated through the back diode with red modulated light and the optical bias applied onto the front diode.

From the experimental results it is observed that when using a red modulated light the thin a-SiC : H front absorber (200 nm) maximizes the conversion efficiency for blue front optical bias and the thickest back absorber layer (1000 nm) minimizes the conversion efficiency in the red range.

Results show that the conversion efficiency to a red modulated light under blue front optical bias is maximized when a 200 nm a-SiC : H front absorber is used, and minimized in the red range if the absorber layer of the back diode is around 1000 nm thick. In those devices the green photons absorption occurs mainly across the front diode, the n–p defectous interface and at the front side of the back diode. Under reverse bias and blue irradiation the collection is high since the back diode becomes fully depleted due to its self-biasing process. Under red illumination the a-Si:H back absorber acts as a load due to the high light penetration depth of the red photons and the low collection is determined by the dark characteristics of the front diode. In the green spectral range the reverse bias increases the potential drop across the back diode and the collection increases linearly. The effect of the applied voltage on the color selectivity and spectral sensitivity is discussed and supported by a physical model based on a numerical simulation.

FINE-TUNING OF THE SPECTRAL COLLECTION EFFICIENCY IN MULTILAYER JUNCTIONS

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a-SiC:H/a-Si:H p-i-n/p-i-n tandem cells with different i-layer thickness have been produced by PECVD and tested for a proper fine-tuning of the spectral collection efficiency. The tandem structure takes advantage on the radiation wavelength selectivity due to the different light penetration depth inside the a-Si:H and a-SiC:H absorbers. The thickness and the absorption coefficient of the front p-i-n cell were optimized for blue collection and red transmittance and the thickness of the back one adjusted to achieve full absorption in the green and high collection in the red spectral ranges. Preliminary results show that device optimization for red detection can be obtained by reducing the thickness of the internal recombination junction while by increasing the intrinsic layer of the bottom a-Si:H cell, a better detection of the green color under appropriated applied voltages is foreseen.

The physics behind the device functioning is explained through a numerical simulation of the internal electrical configuration of the device in dark and under different wavelength irradiations. Considerations about conduction band offsets, electrical field profiles and inversion layers will be taken into account to explain the optical and voltage bias dependence of the spectral response. Experimental results about the spectral collection efficiency are presented and discussed from the point of view of the color sensor applications.

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A GENERIC NETWORK-ON-CHIP ARCHITECTURE FOR RECONFIGURABLE SYSTEMS: IMPLEMENTATION AND EVALUATION

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The design of electronic systems in a System-on-Chip (SoC) depends on the reliable and efficient interconnection of many different components. The Network-on-Chip (NoC) is a scalable communication infrastructure able to tackle the communication needs of future SoC. However, routers of a NoC introduce a relative area overhead and increase the average latency. Therefore, in the design process it is important to consider mechanisms to improve area and performance of NoC infrastructures. In this paper, we propose a generic NoC architecture that can be tailored to the specific requirements of the system looking to improve area usage, average communication latency and throughput. An extensive analysis and tests of the proposed architecture have been performed to evaluate the approach.

APPLICATION SPECIFIC INSTRUCTION SET PROCESSOR FOR ADAPTIVE VIDEO MOTION ESTIMATION

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Motion estimation is the most demanding operation of a video encoder, corresponding to at least 80% of the overall computational cost. With the proliferation of portable handheld devices that support digital video coding, data-adaptive motion estimation algorithms have been required to dynamically configure the search pattern not only to avoid unnecessary computations and memory accesses but also to save energy. This paper proposes an Application Specific Instruction Set Processor (ASIP) to implement data-adaptive motion estimation algorithms, that is characterized by a specialized data-path and minimum and optimized instruction set. Due to its low-power nature, this architecture is specially adequate to develop motion estimators for portable, mobile and battery supplied devices. A cycle-based accurate simulator was also developed for the proposed ASIP and fast and data-adaptive search algorithms have been implemented, namely, the four-step search and the motion vector field adaptive search algorithms. Based on the proposed ASIP and the considered adaptive algorithms, several motion estimators were synthesized in 0.13µm CMOS technology. Experimental results show that very-low power adaptive motion estimators have been achieved to encode QCIF video sequences.

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IEEE Computer Society, August 2006, Pages 160-167
9th EUROMICRO Conference on Digital System Design: Architectures, Methods and Tools (DSD 2006)

AREA AND PERFORMANCE OPTIMIZATION OF A GENERIC NETWORK-ON-CHIP ARCHITECTURE

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Publicado em:
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Complex Systems-on-Chip (SoC) with multiple interconnected stand--alone designs require high scalability and bandwidth. Net-work-on--Chip (NoC) is a scalable communication infrastructure able to tackle the communication needs of these SoCs. In this paper, we consider the optimization of a generic NoC to improve area and performance of NoC based architectures for dedicated applications. The generic NoC can be tailored to an application by changing the number of routers, by configuring each router to specific traffic requirements, and by choosing the set of links between routers and cores. The optimization algorithm determines the appropriate NoC and routers configuration to support a set of applications considering the optimization of area, and performance. The final solution will consist of an heterogeneous NoC with improved quality. The approach has been tested under different operating conditions assuming implementations on an FPGA.

FEEDBACK CHANNEL IN PIXEL DOMAIN WYNER-ZIV VIDEO CODING: MYTHS AND REALITIES

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Wyner-Ziv (WZ) video coding – a particular case of distributed video coding (DVC) – is a new video coding paradigm based on two major Information Theory results: the Slepian-Wolf and Wyner-Ziv theorems. Recently, practical WZ video coding solutions were proposed with promising results. Many of the solutions available in the literature make use of a feedback channel (FC) to per-form rate control at the decoder. In this context, this paper intends to analyse the impact of this feedback channel, notably through a number of metrics such as the frequency the feedback channel is used as well as its associated rate. It is also presented a study on the evolution of the decoded frames quality as more parity bits are requested via feedback channel. Those measures are important since they allow characterizing the usage of the feedback channel, and have never been presented in the literature.

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14th European Conference Signal Processing Conference, Florence, Italy, September 2006

LOW POWER DISTANCE MEASUREMENT UNIT FOR REAL-TIME HARDWARE MOTION ESTIMATORS

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Int. Workshop on Power and Timing Modeling, Optimization and Simulation (PATMOS 2006)

Real-time video encoding often demands hardware motion estimators, even when fast search algorithms are adopted. With the widespread usage of portable handheld devices that support digital video coding, low power consideration becomes a central limiting constraint. Consequently, adaptive search algorithms and special hardware architectures have been recently proposed to perform motion estimation in portable and autonomous devices. This paper proposes a new efficient carry-free arithmetic unit to compute the minimum distance in block matching motion estimation. The operation of the proposed unit is independent of the adopted search algorithm and of the used prediction error metric, simultaneously speeding up motion estimation and significantly reducing the power consumption. Moreover, its low latency is particularly advantageous when partial distance techniques are applied to further reduce the power consumption. Experimental results show that the proposed unit allows to reduce the computation time in about 40% and it consumes 50% less power than commonly adopted architectures.

VALIDATION OF A NOVEL VEHICULAR MOBILITY MODEL FOR WIRELESS NETWORKS

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ABSTRACT

In this paper a novel realistic vehicular mobility model is validated. It captures the moving-in-groups, conscious traveling, and introduces the concept of smart traveling while following drivers' social behavior extracted from inquiries and experimental traffic measurements. Under the model, a routing algorithm is considered. The routing algorithm minimizes the distance to a target on a step by step form, in every street crossing. This is done under a hierarchic street level structure that optimizes travel speed and quality.

The mobility model was simulated and validated in a real mobility scenario using, as case study, the city of Lisbon. The correlation values (between simulated data and theoretical distributions), arrival to destination success rate and directional statistics produced satisfactory results.

The model concept is perfectly generic and applicable to other locations, provided that the corresponding street database and vehicular traffic information are available.

The model outputs several parameters, including sinuosity indicator and traffic load. The sinuosity indicator is a powerful parameter on the characterization of urban radio environments when mobility is used in wireless networks simulation. Vehicular traffic load analysis is also presented. It can be used in further work over wireless traffic modeling, on a street segment basis or on a AU (Analysis Unit) perspective.

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9th International Symposium of Wireless Personal Multimedia Communications 2006, San Diego, EUA, 17-21 de Setembro de 2006

EVALUATION OF AN LPR-BASED TOLL ENFORCEMENT SYSTEM ON PORTUGUESE MOTORWAYS

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This paper presents an approach for evaluating video-based enforcement systems for motorway toll collection, which has been applied to the case of Portugal's largest motorway operator, Brisa. The results of this evaluation have contributed to the design of a new LPR system, denoted advanced license plate recognition (ALPR), also described in this paper. The ALPR is currently being deployed not only by Brisa, but also by other operators that use the Via Verde system. A significant decrease in the need for human intervention has been an important improvement, in which the introduction of a tunable and trustable confidence level in the LPR process has played a key part.

AN INSIGHT INTO WIDEBAND DIRECTIONAL CHANNEL MODELS

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ABSTRACT

In this paper an overview of the work performed in what refers to directional channel modeling, is presented.

Different types of channel models are approached: geometrical, parametrical and correlation oriented. The set of focused directional channel models is not system-specific. Some of these models were derived from previously known models, with the extension of the directional information, or were developed to maintain compatibility with them.

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YBRID KNOWLEDGE MODELING FOR AMBIENT INTELLIGENCE

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This paper describes our research in enhance everyday devices as a solution to adapt Spoken Dialogue Systems (SDS) within ambient intelligence. In this context, a SDS enables universal access to ambient intelligence for anyone, anywhere at anytime, allowing the access to any device through any media or language. The main problem that we want to address is the spontaneous configuration of SDS to deal with a set of arbitrary plug and play devices. Such problem is resumed as a portability feature and is a critical research issue. We propose a hybrid approach to design ubiquitous domain models to allow the SDS to recognize on the fly the available devices and tasks they provide. When a device is activated or deactivated, a broker's knowledge model is updated from device's knowledge model using a knowledge integration process. This process was tested in the home environment represented by a set of devices.

CONTENT ADAPTIVE WYNER-ZIV VIDEO CODING DRIVEN BY MOTION ACTIVITY

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In distributed video coding (DVC), the video statistics are exploited, partially or totally at the decoder. A particular case of DVC, Wyner-Ziv video coding deals with lossy source coding with side information at the decoder and allows moving part or the entire motion estimation task to the decoder. In this context, it is the decoder responsibility to obtain the side information, a guess of the encoded Wyner-Ziv frame and the encoder only sends parity bits to improve its quality. In this paper, a technique targeting the improvement of the quality of the side information, and thus of the rate-distortion performance of the Wyner-Ziv codec is proposed. This is achieved by adaptively adjusting the size of the motion interpolation structure (or GOP length) according to the motion activity along the sequence. Experimentally, this allows to achieve gains up to 0.8 dB without performing any motion estimation or complex mode decision at the encoder.

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HYBRID DISTRIBUTED VIDEO CODING USING SCA CODES

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IEEE International Workshop on Multimedia Signal Processing, Victoria, Canada, October 2006

We describe the architecture for our distributed video coding (DVC) system. Some key differences between our work and previous systems include a new method of enabling decoder motion compensation, and the use of serially concatenated accumulate syndrome codes for distributed source coding. To evaluate performance, we compare our system to the H.263+ and H.264/AVC video codecs. Experiments show that our system is comparable to DVC systems from Stanford and Berkeley in the sense that our system performs better than H.263+ Intra, but worse than H.263+Inter and H.264/AVC.

EXTENDING .NET REMOTING WITH DISTRIBUTED GARBAGE COLLECTION

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

Current DGC solutions are either not safe, not complete or not portable to widely used platforms such as .NET. As a matter of fact, most solutions either run on specialized environments or require modifications of the underlying virtual machine (e.g. Rotor) hindering its immediate utilization.

This paper describes the architecture, implementation and performance measurements of a DGC algorithm that: i) is capable of reclaiming both acyclic and cyclic garbage, while ii) being portable in the sense that it does not require the underlying virtual machine to be modified.

The distributed garbage collector was implemented on top of two realizations of the Common Language Infrastructure (.NET virtual machine specification): Common Language Runtime (CLR) and Shared Source CLI (SSCLI), commonly known as Rotor. The implementation requires no modification of the environment, it makes use of the aspect-oriented functionalities provided, and the preliminary results are encouraging.

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Proceedings of the Second Edition of the International Conference on Innovative Views of NET Technologies, October 2006

02

A DOMAIN KNOWLEDGE ADVISOR FOR DIALOGUE SYSTEMS

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This paper describes ongoing research in order to enhance our Domain Knowledge Manager (DKM) that is a module of a multi propose Spoken Dialogue System (SDS) architecture. The application domain is materialized as an arbitrary set of devices, such as household appliances, providing useful tasks to the SDS users. Our main contribution is a DKM advisor service, which suggests the best task device pairs to satisfy a request. Additionally, we also propose a DKM recognizer service to identify the domain's concepts from a natural language request. These services use as knowledge source a domain model, to obtain knowledge about devices and the tasks they provide. The implementation of these services allows the DKM to provide a high level and easy to use small interface, instead of a conventional service interface with several remote procedures/methods. These services have been tested into a domain simulator. Our contributions try to reach SDS domain portability issues.

COLOUR FILTERING IN A-SIC:H BASED P-I-N-P-I-N CELLS: A TRADE-OFF BETWEEN BIAS POLARITY AND ABSORPTION REGIONS

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A large area colour imager optically addressed is presented. The colour imager consists of a thin wide band gap p-i-n a-SiC:H filtering element deposited on the top of a thick large area a-SiC:H(-p)/a-Si:H (-i)/a-SiC:H(-n) image sensor, which reveals itself an intrinsic colour filter. In order to tune the external applied voltage for full colour discrimination the photocurrent generated by a modulated red light is measured under different optical and electrical bias. Results reveal that the integrated device behaves itself as an imager and a filter giving information not only on the position where the optical image is absorbed but also on it wavelength and intensity.
The amplitude and sign of the image signals are electrically tuneable. In a wide range of incident fluxes and under reverse bias, the red and blue image signals are opposite in sign and the green signal is suppressed allowing blue and red colour recognition. The green information is obtained under forward bias, where the blue signal goes down to zero and the red and green remain constant. Combining the information obtained at this two applied voltages a RGB colour image picture can be acquired without the need of the usual colour filters or pixel architecture. A numerical simulation supports the colour filter analysis.

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Sensors and Actuators A: Physical Volume 132, Issue 1, 8 November 2006, Pages 218-223 The 19th European Conference on Solid-State Transducers

A REAL TIME COLOUR AND IMAGE PROCESSING PIN-PIN DEVICE WITH OPTICAL READOUT

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Revista Mexicana de Fisica 52 (2 SUPPL.), 2006, pp. 79-82

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

The various design parameters and addressing architecture tradeoffs are discussed. The influence on the transfer functions of an a-SiC:H sensing absorber optimized for red transmittance and blue collection or of a floating anode in-between is analysed. Results show that the thin a-SiC:H sensing absorber confines the readout to the switching diode and light filters the structure allowing full colour detection at two appropriated voltages. When the floating anode is used the spectral response broadens allowing B&W image recognition with improved light-to-dark sensitivity. A physical model supports the image and colour recognition process.

LARGE AREA P-I-N FLEXIBLE IMAGE SENSITIVE DEVICES DEPOSITED ON PLASTIC SUBSTRATES

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Large area p-i-n image sensors deposited on plastic substrates were produced at low temperatures (110 ºC) 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 on 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 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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Revista Mexicana de Fisica 52 (2 SUPPL.), 2006, pp. 57-60

THIN FILM SENSORS PRODUCED AT LOW TEMPERATURES: A TRADE-OFF BETWEEN CARBON COMPOSITION AND SPECTRAL RESPONSE

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Publicado em:
Revista Mexicana de Fisica 52 (2 SUPPL.), 2006, pp. 32-35

A series of large area single layers and homo and heterojunction cells in the assembly glass/ZnO:Al/p (SixC1-x:H)/i (Si:H)/n (SixC1-x:H)/Al (o‹x‹1) were produced by PE-CVD at low temperature. Junction properties, carrier transport and photogeneration are investigated from dark and illuminated current-voltage characteristics, and spectral response measurements in dark and under different illumination conditions. For the heterojunction cells atypical J-V characteristics under different illumination conditions are observed leading to poor fill factors. High series resistances around 106 W were measured. In these structures it was observed that the responsivity decreases with the increase of the light bias intensity. The homojunction presents the typical behaviour of a non optimised p-i-n cell and the responsivity varies only slightly with the light bias conditions.

RESOLUTION OF MAXWELL'S EQUATIONS IN A NON STAGGERED GRID MODEL

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In this paper a scheme to obtain an adaptive method in space for the resolution of Maxwell's equations is presented. Using interpolating wavelets it is possible to obtain an adaptive grid allowing a reduction of the computation time and an economy of the computational resources. Using the not staggered grid model the stability factor is improved when compared with the classic FDTD and its value is great that one. This factor is more limited with the increase of the interpolating polynomial. On the other hand the dispersion proprieties are more restricted, when compared with a model of staggered grid.

Publicado em:
EUCAP2006, Nice, França, 06 a 10 de Novembro 2006

MAXIMUM ENTROPY MOTIVATED GRAPHEME-TO-PHONEME, STRESS AND SYLLABLE BOUNDARY PREDICTION FOR PORTUGUESE TEXT-TO-SPEECH

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Publicado em:
IV Biennial Workshop on Speech Technology, Zaragoza, Espanha, 8-10 Novembro 2006

In this paper we present a framework for grapheme-to-phoneme (G2P) conversion, stress and syllable boundary prediction for European Portuguese (EP) Text-to-Speech (TTS) Systems. For all prediction tasks Maximum-Entropy models were used for classification. Due to the need of expensive work by experts to implement rule based G2P converters there was interest in developing probabilistic models with the Maximum-Entropy approach to solve the previous mentioned symbolic pre-processing within a TTS system. The system presented in this work is a fast and flexible approach which gives good results in each of the prediction tasks, optimal for fast application development in the TTS domain. The data used for training the G2P conversion model is manually labelled from continuous speech with natural vocalic reduction and co-articulation between words effects, common in Portuguese continuous speech. The framework is used for EP but is also usable for Brazilian Portuguese (BP) where minor changes have to be done in the G2P training data whereas stress and syllable models are the same.

BIAS SENSITIVE SPECTRAL SENSITIVITY IN DOUBLE A-SIC: H PIN STRUCTURES

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In this work we discuss the use of multilayer stacked structures (p(SiC:H)/i(SiC:H)/n(SiC:H)/p(SiC:H)/i(Si:H)/n(Si:H)) sandwiched between two transparent conductive contacts as colour sensing devices. The thickness and the absorption coefficient of both front and back p–i–n cells were specifically designed in order to achieve simultaneously high blue collection and red transmittance in the front cell and full green absorption and high red collection in the back cell. Electric and optical sensing methods were used for measuring the current–voltage characteristics and the spectral sensitivity, under different experimental conditions. Results show that the spectral sensitivity of the device is strongly modulated by the applied voltage, which allows colour selectivity. The results were supported by a physical model.

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PARALLEL BAYESIAN CODE DELAY AND DOPPLER FREQUENCY ESTIMATION IN GNSS RECEIVERS

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Proceedings of 3rd ESA Workshop on Satellite Navigation User Equipment Technologies – NAVITEC 2006, December 11-13, ESA/ESTEC, Noordwijk, The Netherlands.

The operation of conventional GNSS receivers is based on two closed loops (delay-lock and phase/frequency-locked loops) for the tracking of code delay and Doppler frequency. Although this architecture performs well with rectangular pulses (such as the legacy GPS) it is clearly sub-optimal when it operates with more complex pulses like those found in Binary Offset Carrier (BOC) modulation, which will be used in Galileo and modernized GPS. In fact, the BOC waveforms have multi-peaked autocorrelation functions that lead to potential tracking ambiguities (i.e., false locking). Techniques to mitigate this problem have been suggested at the cost of increased receiver complexity (for instance, bumpjumping). Following the same framework used in a previous paper by the authors for the problem of acquisition in high-lymanoeuvrable receivers, we propose herein a state-space model--based (Bayesian) approach to the problem of code and phase/frequency tracking. The solution consists of modeling the phase, frequency and amplitude of the incoming signal as components of a state vector and using a bank of similar stochastic nonlinear filters (for instance, extended Kalman filters) to track them. The filters are fed with the correlators outputs, where code replicas with different delays are used. At each iteration, the code delay estimates are obtained from the nonlinear filter with the largest amplitude estimate. The reason for this is that, since the correlators outputs depend on the signal autocorrelation, the output with the smallest code delay error will exhibit the largest amplitude. During the receiver operation the ranges of the code delay and the Doppler frequency are periodically adjusted in order to avoid losing tracking. In this paper special attention will be devoted to the application of the proposed receiver to BOC(1,1) given the importance of this modulation in Galileo and modernized GPS, namely in band L1.

STROBE CORRELATOR DESIGN FOR MULTIPATH MITIGATION IN BOC GNSS RECEIVERS

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The concept of strobe correlator receiver for GNSS (Global Navigation Satellite System) signals was considered by several authors. It consists of correlating the inphase and quadrature components of the incoming signal with a locally generated spreading code and a gating sequence. The gating signal is a train of specially tailored strobe pulses locked with the code sequence. The strobe pulse is characterized by its duration and shape. By carefully selecting the strobe pulse, different performances can be obtained in terms of robustness to thermal noise, multipath mitigation capability, and code acquisition range. Besides, the approach is very powerful as most conventional delay lock loops (DLL), such as the early-late and the double-delta DLL, are particular cases of a strobe correlator, as shown, before. Binary Offset Carrier (BOC) signals have found application in modernized GPS (M-signal) and in Galileo. The interest in BOC modulations stems from the advantages they offer regarding the conventional binary PSK (BPSK) modulation, namely better tracking performance and interference mitigation. It was shown that the concept of DLL based on bipolar symmetrical strobe pulses could be extended to BOC(m, n) signals. Although the proposed solution presents an extra degradation due to thermal noise, this drawback is compensated by the superior performance in multipath scenarios. The bipolar symmetrical strobe pulse utilized therein has been previously applied by several authors in the processing of GPS C/A signals to mitigate multipath. This is an ad hoc solution, since no optimality criterion was considered in the design of the pulse. The use of asymmetrical strobe pulses to reduce multipath errors was suggested for GPS C/A signals. In a previous work, a new approach approach to the design of asymmetrical strobe pulses for BOC signals is proposed. A target code discriminator response with desirable characteristics is defined, allowing to determine the strobe pulse as the solution of an integral equation. Since this problem is rather complicated, several shortcuts, that permit to obtain approximated solutions with small computational effort, are presented. The resulting pulse provides good multipath mitigation capability, extended code tracking range, and lack of false code lock points. The pur-

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pose of the present paper is to analyze the performance improvement that results from considering asymmetrical strobe pulses for the tracking of BOC signals in terms of robustness to thermal noise, loss of tracking and capability to mitigate multipath. Following the previous work, we started with a pre-defined (target) code discriminator response with suitable characteristics in terms of code tracking range and multipath mitigation capability and, taking into account the constrains, solved an integral equation whose solution is the desired strobe pulse. Those solutions are analyzed and compared with the standard techniques and simulation results are presented.

COORDINATION WITH COLLECTIVE AND INDIVIDUAL DECISIONS

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The response to a large scale disaster, e.g. an earthquake or a terrorist incident, urges for low-cost policies that coordinate sequential decisions of multiple agents. Decisions range from collective (common good) to individual (self-interested) perspectives, intuitively shaping a two layer decision model. However, current decision theoretic models are either purely collective or purely individual and seek optimal policies. We present a two layer, collective versus individual (CvI) decision model and explore the tradeoff between cost reduction and loss of optimality while learning coordination skills. Experiments, in a partially observable domain, test our approach for learning a collective policy and results show near optimal policies that exhibit coordinated behavior.

Publicado em:
Progress in Artificial Intelligence, IBERAMIA-SBIA-06, Volume 4140 of Lecture Notes in Artificial Intelligence, Pages 37-47, Springer-Verlag. 2006.

A SYSTEM TO CAPTURE, SHARE AND ACCESS PERSONAL MEMORIES

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Publicado em:
In Memories for life Colloquium, London, (2006).

This paper presents a system to access personal memories composed by digital pictures. The system consists of a retrieval engine, a desktop interface to share personal memories and a mobile user interface that allows capture and automatic annotation of images. The retrieval engine uses Global Positioning System (GPS) location data, low-level visual features and semantic concepts previously trained to retrieve images. With the mobile interface people can capture, share personal pictures and navigate in the physical space when visiting historical sites, museums and other touristic activities using their Personal Digital Assistants (PDA). The visitors can take photos and submit them to the system to receive contextually related photos taken by others or themselves. Experimental results are presented to show the performance of the retrieval mechanisms and the usefulness of the navigation system.

PHOTO RETRIEVAL FROM PERSONAL MEMORIES USING GENERIC CONCEPTS

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This paper presents techniques for retrieving photos from personal memories collections using generic concepts that the users specify. It is part of a larger project for capturing, storing, and retrieving personal memories in different contexts of use. Semantic concepts are obtained by training binary classifiers using the Regularized Least Squares Classifier (RLSC) and can be combined to express more complex concepts. The results that were obtained so far are quite good and by adding more low level features, better results are possible. The paper describes the proposed approach, the classifier and features, and the results that were obtained.

Publicado em:
Advances in Multimedia Information Processing - PCM 2006, Springer LNCS, vol. 4261, pp. 633-640, 2006.

GERAÇÃO DE FORMULÁRIOS WEB COM BASE EM TEMPLATES INFOPATH

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Publicado em:
XATA2006 — XML: Aplicações e Tecnologias Associadas, Portalegre, Fevereiro de 2006.

A aplicação InfoPath, pertencente ao conjunto de ferramentas de escritório Microsoft Office, tem por função o desenho e preenchimento de formulários associados a documentos XML. Contudo, os cenários de utilização destes formulários são limitados, porque a fase de preenchimento requer o uso da aplicação InfoPath e o acesso directo às fontes de dados.

O presente artigo descreve aspectos do desenho e implementação do sistema WebInfoPath (WIP), que tem como objectivo a geração e suporte à execução de formulários web para a visualização e recolha da informação e ligação às fontes de dados. Estes formulários são gerados com base em templates definidos através da aplicação InfoPath. Define-se uma arquitectura expansível para este objectivo e descrevem-se aspectos da sua implementação, nomeadamente: gerador de páginas e controlos ASP.NET; biblioteca de classes para suporte à execução; e forma de integração em aplicações web.

ON THE USE OF INDEPENDENT COMPONENT ANALYSIS FOR IMAGE COMPRESSION

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This paper addresses the use of independent component analysis (ICA) for image compression. Our goal is to study the adequacy (for lossy transform compression) of bases learned from data using ICA. Since these bases are, in general, non-orthogonal, two methods are considered to obtain image representations: matching pursuit type algorithms and orthogonalization of the ICA bases followed by standard orthogonal projection.

Several coder architectures are evaluated and compared, using both the usual SNR and a perceptual quality measure called picture quality scale. We consider four classes of images (natural, faces, fingerprints, and synthetic) to study the generalization and adaptation abilities of the data-dependent ICA bases. In this study, we have observed that: bases learned from natural images generalize well to other classes of images; bases learned from the other specific classes show good specialization. For example, for fingerprint images, our coders perform close to the special-purpose WSQ coder developed by the FBI. For some classes, the visual quality of the images obtained with our coders is similar to that obtained with JPEG2000, which is currently the state-of-the-art coder and much more sophisticated than a simple transform coder.

We conclude that ICA provides an excellent tool for learning a coder for a specific image class, which can even be done using a single image from that class. This is an alternative to hand tailoring a coder for a given class (as was done, for example, in the WSQ for fingerprint images). Another conclusion is that a coder learned from natural images acts like an universal coder, that is, generalizes very well for a wide range of image classes.

Publicado em:
Signal Processing: Image Communication, vol. 21, n.º 5, pp. 378-389, June 2006.

TEACHING CLASSICAL CONCURRENT ALGORITHMS USING A GRAPHICAL INTERFACE TOOLKIT - SesTools

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The study of classical concurrent algorithms like Readers/Writers is a key concept on every Operating Systems subject. In this paper we present a graphical tool (SesTools) developed on top of the Windows Operating System in order to help students to understand better these algorithms. We also present the conclusions that we have achieved in the scope of the Operating Systems of the Informatics and Computers Engineering curricula at Instituto Superior de Engenharia de Lisboa (ISEL).

Publicado em:
VII Congreso TAEE "Tecnologías Aplicadas a la Enseñanza de la Electrónica – Technologies Applied to Electronics Teaching", Madrid, Spain, July 2006. (apresentado em poster)

MIGRATING FROM A WEB SITE TO A MOODLE BASED CMS

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This paper presents the results of a work made to demonstrate the advantages of adopting a course management system versus a pure web site for teaching aid. It presents the lessons learned during the process of migrating already existing web contents to learning objects organized in SCORM content packages. The adoption of MOODLE as a concrete free CMS for publishing the migrated contents is reported. Finally, the use of the system for continuous students' performance evaluation and other teaching activities are mentioned.

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VII Congreso TAEE "Tecnologías Aplicadas a la Enseñanza de la Electrónica – Technologies Applied to Electronics Teaching", Madrid, Spain, July 2006.

NFC TECHNOLOGIES IN MOBILE PHONES AND EMERGING APPLICATIONS

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Publicado em:
7th IFIP "International Conference on Information Technology for Balanced Automation Systems in Manufacturing and Services", 4–6 September, Niagara Falls, Ontario Canada.

The main purpose of this paper is to introduce some new non-conventional applications to allow the exploitation of today's mobile phone resources, namely their connectivity capabilities to other devices.
There is a great potential for applications to take advantage of these available resources, to perceive and interact with the world around us, namely to serve as a user interface to interact with controlled devices. Recently beyond the necessary speaker and microphone, cell phones incorporate more sensing, processing and storage capabilities as well as alternative communication systems, e.g. digital camera, Bluetooth. This paper addresses, in particular, the Near Field Communication (NFC) incorporated in cell phones and enumerates some of its main promising applications like in device monitoring and control.

NEW DATA PREPARATION PROCESS – A CASE STUDY FOR AN EXOMARS DRILL

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This paper addresses the data preparation process for a drill fuzzy monitoring tool. The objective is to describe how to automatically generate fuzzy variables, for a drill monitoring system, using inferred nominal values and their dispersion for each variable. Here, we focus on the knowledge discovery tasks that encompass data extraction, data cleaning, data transformation and then the construction of the fuzzy variables.

Publicado em:
World Automation Congress (WAC2006), Hungary.

MONITORING & DIAGNOSIS ON-BOARD SOFTWARE MODULE FOR MARS DRILLER (MODI)

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In this paper we first present the concept of Monitoring & Diagnosis techniques for remote systems within the context of robotic Martian exploration. Then we show how the MODI project is aiming at monitoring and diagnosing a drill and sampling system for Martian exploration rover, and explain how MODI implements a fuzzy system to monitor and diagnose a drill. Last, we present the preliminary test results of MODI and demonstrate that MODI allows monitoring mileage of the drill and preventing dramatic failures, hence extending the drilling operations capability of a Martian rover in the long term.

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IWPSS 2006 Proceedings "5th International workshop on Planning and Scheduling for Space", October 22–25, 2006, Baltimore, USA, http://www.stsci.edu/institute/conference/iwpss/plenary-01-Jameux.pdf.

02

THERMALIZATION AND RECOMBINATION IN EXPONENTIAL BAND TAIL STATES

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We present an analytical model that combines the complementary experimental evidence of spatial dispersion (DAP recombination) and energetic dispersion (band tails). The model describes the competition between thermalization and recombination of excess carriers trapped in exponentially distributed (in energy), discrete localized (in space) states. We use the energy dependence of the relaxation rates to derive the energy and time dependence of sub gap photoluminescence. The model predicts that the yellow luminescence band (YLB) and blue luminescence band (BLB) commonly observed in GaN are not separate entities, but reflect the competition of thermalization and recombination. A distinct kink is observed in transient PL in the microsecond range, in the limiting cases of strong tailing and/or low temperatures, indicating the transition from thermalization-limited to (radiative) recombination-limited excess carrier relaxation. Both prediction are in line with experiment, and able to resolve interpretational difficulties.

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phys. stat. sol. (c) 3, No. 6, 1637–1644 (2006).

DIFFUSION LENGTHS IN GAN OBTAINED FROM STEADY STATE PHOTOCARRIER GRATINGS (SSPG)

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Publicado em:
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We present diffusion length measurements in gallium nitride (GaN) and AlXGa1–XN/GaN multilayers with aluminium contents up to Xmax = 37 at.%. The opto-electrical method employed is the steady-state photocarrier grating (SSPG), which uses two interfering laser beams to induce a periodic resistivity modulation normal to the sense current lines. We experimentally refined the SSPG, using a double beamsplitter technique and introducing a variable ND filter. We measured diffusion lengths of single GaN and AlXGa1–XN/GaN double layers, and analysed the obtained diffusion lengths as function of the aluminium concentration, comparing them with the respective drift lengths. Finally, we critically discuss the common interpretation in terms of ambipolar transport. We suggest a new model in which minority carriers are rapidly trapped in acceptor-like valence band tails and participate in the grating blurring passively, as spatially localized recombination centres.

NEW RESULTS ON DIFFUSION LENGTHS MEASUREMENTS IN WIDE BANDGAP SEMICONDUCTORS, OBTAINED FROM STEADY STATE PHOTOCARRIER GRATINGS (SSPG)

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In this work we develop our previous measurements of diffusion lengths in gallium nitride using the steady-state photocarrier grating (SSPG) method. We show how the use of a monomode HeCd laser as well as a photoelectrical compensation scheme improves significantly the measurement, and demonstratethe ruggedness of the SSPG technique as well as the reliability of the obtained diffusion length, whichis typically in the range of several hundreds of nanometers. The small-signal photocurrent decay is exponential, with decay times in the millisecond range, a clear indication of trap-limited dynamics. We use the photocarrier grating field quenching to estimate the majority carrier drift mobility. Finally, a thermalization-limited diffusion mechanism is proposed in order to overcome a serious conflict between the experimental data and the recombination-limited SSPG diffusion theory.

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UNSUPERVISED HYPERSPECTRAL UNMIXING

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Publicado em:
Dissertação para obtenção do Grau de Doutor em Engenharia Electrotécnica e de Computadores, Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal

This thesis addresses hyperspectral unmixing, which is the decomposition of pixel spectra acquired by spectral sensors into a collection of constituent spectra, or endmember spectral signatures, and their corresponding abundance fractions. The need for hyperspectral unmixing has been fostered by the development of extremely powerful hyperspectral sensors, with hundreds of narrow (on the order of 10*nm*) contiguous bands, spanning the visible, the near-infrared, and the mid-infrared wavelengths (between 0.3µ*m* and 2.5µ*m*) of the electromagnetic spectrum. These sensors have improved the recognition of Earth substances based on their signatures, *i.e.*, based on the scattered electromagnetic energy on each wavelength. However, since the spatial resolution of any sensor is finite, those substances are very often spatially mixed. In given circumstances, these substances can be unmixed and thus resolved without increasing the spatial resolution of the sensor. This thesis introduces three new methodologies playing relevant roles in the hyperspectral unmixing processing chain. The first method, termed *hyperspectral signal identification by minimum error* (HySime), estimates the signal subspace to reduce the dimensionality of the data to be processed. Since the number of components of hyperspectral vector is large (typically more than 200 bands) and the dimension of the signal subspace is often much smaller, dimensionality reduction leads to reductions in memory requirements and gains in the signal-to-noise ratio.

The second method, termed *vertex component analysis* (VCA), extracts the endmembers exploiting the fact that the spectra of pure pixels are in vertices of a simplex. VCA searches for these vertices based on the assumption that at least one pure pixel per endmember is present in the data set. VCA achieves state-of-the-art performance with a computational complexity between one and two orders of magnitude lower than the best algorithms.

The third method, termed *dependent component analysis* (DECA), formalizes spectral unmixing as a maximum likelihood (ML) problem. DECA uses the expectation maximization (EM) framework to infer the unmixing matrix. The abundance fraction densities are modeled by a

mixture of Dirichlet densities, thus modeling the statistical dependence normally found in hyperspectral data. Compared with VCA, DECA does not need to assume the presence of pure pixels in the observations.

Independent component analysis (ICA) and *independent factor analysis* (IFA) have been used by many authors to unmix hyperspectral data. Due to physical constraints ever present in hyperspectral data, the ICA and IFA central assumption of source statistical independence does not hold. The impact of this source statistical dependence is addressed. It is concluded that ICA and IFA algorithms do not correctly unmix hyperspectral data. We give evidence that the unmixing matrix minimizing the mutual information might be far from the true one.

A set of tests with simulated and real hyperspectral data evaluates the performance and illustrates the effectiveness of the proposed methods.


03

ENGENHARIA MECÂNICA

Anuário Científico 2006

ISEL

I-MERC: A MOBILE ROBOT TO DELIVER MEALS INSIDE HEALTH SERVICES

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With the aim of increasing the quality of the meals transportation service inside hospitals and health care centers (HHCC), we are developing a dedicated mobile robot to perform this service, the i-MERC. This robot is equipped with a heating system in the meals compartment which guarantees the meals temperature and prevents bacteriologic proliferation. The i-MERC also integrates a personalized diets information system where information about patients' diets can be introduced and accessed by the service personnel. This project has been developed within the compass of the Master in Engineering Design, at the Technical University of Lisbon. The product development of the robot addressed many knowledge areas, some of which are presented in this paper. We finished the first stage of the project with a service concept, a virtual prototype which included some key specifications and a physical prototype. Presently, we are continuing the product development and searching some stakeholders that would be interested in the project.

Publicado em:
2ª IEEE Internacional Conference on Cibernetics & Intelligence Systems & Robotics, Automation & Mechtronics, Bangkok, Tailândia, Junho de 2006.

A DESIGN APPROACH FOR THE DEVELOPMENT OF A DEDICATED MEALS TRANSPORTER MOBILE ROBOT

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Publicado em:
5th International Conference in Mechanics & Materials in Design, Porto, Portugal, Julho de 2006.

In this paper we present the design of a dedicated meals transporter mobile robot, motivated by the need to increase the quality of the meals transportation service inside hospitals and health care centres (HHCC). This robot has isolated walls and a heating system which keeps meals temperature at acceptable levels to prevent bacteriologic proliferation. The project has been developed within the compass of the Master in Engineering Design, at the Technical University of Lisbon. The product development addressed many knowledge areas such as project management, geometric modeling, ergonomics, mechanical technology and materials, structural and thermal validation, micro-electronic, control systems, artificial intelligence and communication networks, some of which are presented in this paper. A prototype was developed to be presented to stakeholders that would be interested in the project.

A SYSTEMATIC APPROACH TO COURSE DESIGN AT SUBJECT LEVEL ON A MECHANICAL ENGINEERING COURSE SO AS TO ENCOURAGE ACTIVE LEARNING

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This paper describes the use of cooperative online assignments in tandem with traditional lecture methods in the subject of Energy and the Environment taken by final year Mechanical Engineering students. A systematic approach to course design is presented whereby successive versions of the course were altered incrementally so as to better promote active student learning.

Publicado em:
WSEAS Transactions on Advances in Engineering Education, Issue 6, Vol. 3, June 2006, ISSN 1790-1979, pp.482-487.

PILOT TEST AND THEORETICAL ANALYSIS OF ONE OR MORE COMPONENT FUEL

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The evaporation rate of different liquids is measured by exposing small droplets to an intensive radiative heat load. Three liquids are used namely water, n-heptane and rape seed oil. A mixture of n-heptane and rape seed oil (20/80 vol) is also analysed.
The sample results show the evaporation of different fractions of liquid for different wall temperatures and a constant counter flow of nitrogen.

Publicado em:
Proceedings of Gépészet 2006, Fifth Conference on Mechanical Engineering, May 25-26, Budapest, Hungary.

REMOTELY VISITING ACADEMIC LABS USING ICTs

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This work describes experiences using services offered by the new Information and Communication Technologies (ICTs) and how they may open perspectives for increasing students, teachers and researchers knowledge on lab capabilities and cooperation activities between distant institutions.

The experiences involve the Laboratory of Instrumentation for Measurement (LIM) at Faculdade de Engenharia da Universidade do Porto (FEUP) and the Laboratory of Heat Engines (LHE) of the Department of Energy Engineering (DEE), at the Budapest University of Technology and Economics (BUTE).

The technologies used are based on basic systems for IP voice and video communications: the Skype® software as a free VoIP application and a network camera for capturing and sending live video over an IP network.

The co-operation between the DEE at BUTE and ISEL also involves Universities visiting. It is within the present Cooperation Programme that a Remote Lab Visit was performed with FEUP, followed by a real visit. Later, a Remote Lab Visit was performed with DEE at BUTE.

The simplicity and the realism of the used techniques launched new perspectives on Remote Lab Visits involving all the participants.

Publicado em:
34th SEFI Annual Conference - Engineering Education and Active Students, June 28 – July 1, Uppsala, Sweden.

INCLUDING COOPERATIVE ONLINE LEARNING AT SUBJECT LEVEL ON A MECHANICAL ENGINEERING COURSE

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This paper describes the use of cooperative online assignments in tandem with traditional lecture methods in the subject of Energy and the Environment on the final year of a Mechanical Engineering program so as to encourage active student learning.

Publicado em:
3rd WSEAS/IASME International Conference on Engineering Education (EE'06), 11–13 July, Vouliagmeni, Athens, Greece.

PROMOTING ACTIVE LEARNING IN MECHANICAL ENGINEERING

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In order to promote active learning in a Mechanical Engineering course a learning/teaching methodology which comprises several distributed activities is introduced, hence providing a wider choice and opportunity for students' effective learning. An online collaborative environment is implemented using different technologies, namely a mail box and a discussion forum. This methodology allows students a wider choice and diversity of practices and promotes contact with real world applications, while contributing for students' learning motivation and creativity enhancement.

Publicado em:
Proceedings of IMECE2006, ASME International Mechanical Engineering Congress and Exposition November 5-10, 2006, Chicago, Illinois, USA.

APRENDIZAGEM COLABORATIVA

Carvalho, Isabel S.

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Publicado em:
1ª Conferência Ensino Superior – Desafios e Estratégias, "Bolonha e Práticas Pedagógicas", Escola Superior de Tecnologia de Setúbal, 25-26 Setembro, Setúbal, Portugal (http://ltodi.est.ips.pt/esde/apr-25.htm#)

No âmbito de uma disciplina do 5º ano do curso de Engenharia Mecânica, é proposto aos alunos um modelo de aprendizagem do tipo colaborativo. Este modelo permite a construção de um processo de aprendizagem evolutivo e flexível numa área temática específica. As aulas presenciais decorrem segundo modelos narrativos e interactivos. À estrutura do modelo clássico é adicionada uma componente online que permite uma enorme interactividade entre os alunos ao longo de todo o processo de ensino/aprendizagem.

THE ENGINE OF CREATION: INSPIRATION, DEMATERIALIZATION AND RECOMBINATION

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ABSTRACT

When generating ideas, for example, in a product development process, the way new ideas are put forth is not completely understood, or poorly structured. The present work presents a structured system to better understand the idea generation, i.e. ideation. The author developed a system for creativity characterized by a focused and efficient ideation (both in quantity and quality of the ideas generated). This system has a wide range of application but can also easily be adapted and specialized for different fields of knowledge. It has the ability to create ideas driven or not by the sources of inspiration (market/business, technology and science), resulting in a reactive and proactive potential in an innovation competitive environment. It uses also the most important features of the Creative Templates and Electronic Brainstorming methodologies of creativity, and eliminates their main shortcomings.

Publicado em:
Proceedings do M2D'2006, 5th International Conference on Mechanics and Materials in Design, Porto, Julho de 2006

THE ENGINE OF THE CREATIVE PROCESS: A CONTRIBUTION TO PRODUCT DEVELOPMENT

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Publicado em:
Livro de Artigos da Conferência "Creating and Appropriating Value in Innovation Management", Product Development and Management Association (PDMA), Atlanta, EUA, Outubro de 2006

The ideation generates both useful and useless information. Then, its efficiency is related to the generation of information waste. To increment the ideation efficiency, the author presents a structured system that aims to reduce the generation of information waste, which leads to the improvement of the product development process, both in the product quality and time/cost to market. The reduction of the information waste generated by the engine, leads to a reduction on the control of the process, required to select the best ideas. As a result of this rich information, the flow of information is continuous, and the process is highly flexible in a way to adapt to the competitive environment changes, i.e. information-driven approach. The flexibility of the information-driven process is achieved by an undisciplined/uncontrolled approach, which is difficult to implement, but the authors propose an ideation engine to solve this shortcoming, with a high efficiency and focus. The proposed engine of ideation in combination with the Electronic Brainstorming presents the platform to develop effectively the information-driven process.

MULTIPLE-MODEL FAULT TOLERANT CONTROL OF TERMINAL UNITS OF HVAC SYSTEMS

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In this work, a fault-tolerant control scheme is applied to a air handling unit of a heating, ventilation and air-conditioning system. Using the multiple-model approach it is possible to identify faults and to control the system under faulty and normal conditions in an effective way. Using well known techniques to model and control the process, this work focuses on the importance of the cost function in the fault detection and its influence on the reconfigurable controller. Experimental results show how the control of the terminal unit is affected in the presence a fault, and how the recuperation and reconfiguration of the control action is able to deal with the effects of faults.

Publicado em:
International Symposium on Industrial Electronics, Montreal, Canada, Julho de 2006.

A MULTIPLE-MODEL APPROACH TO MODEL COMPLEX NONLINEAR SYSTEMS.

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Publicado em:
7th Portuguese Conference on Automatic Control, Lisboa, Portugal, Setembro de 2006.

In this paper the multiple-model approach to identify nonlinear complex systems is used. Using a real HVAC system, located at the University of Reading, UK, the multiple-model approach was tested and compared with some nonlinear identification techniques. The known nonlinearities associated to this type of systems are used to test the multiple-model identification algorithms, using a real system. A different switching mechanism is presented, based on optimization algorithms, and compared with different switching approaches.

COMPARISON OF TWO NUMERICAL SOLUTIONS FOR DETERMINATION OF INTERLAMINAR AND CIRCUMFERENTIAL STRESSES IN A COMPOSITE CURVED BEAM

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This paper presents a study of interlaminar tensile and circumferential stress and strain distribution in curved composite beams with a C shape, using the commercial FEM applications LUSAS and ANSYS. A general comparison of results is made between the two FEM applications used. For the circumferential strains in the outer and inner layers, the results are validated with experimental data, obtained from strain gages installed on vacuum bag/autoclave glass/epoxy prepreg beam. The curved beams have a symmetric, non balanced, stacking sequence with a total of 14 layers. The multilayer theory was the basis of the analytical work done (Ko, 1989).

Publicado em:
Artigo apresentado na 5th International Conference on Mechanics and Materials in Design (M2D-2006), publicado no CD-ROM de actas do encontro, 24 a 26 de Julho de 2006, Faculdade de Engenharia da Universidade do Porto, Porto.

DESIGN AND ANALYSIS OF CURVED BEAMS MADE OF COMPOSITE MATERIALS

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Publicado em:
Artigo apresentado na 12th European Conference on Composite Materials (ECCM 12), publicado no CD-ROM de actas do encontro, 29 de Agosto a 01 de Setembro de 2006, Biarritz, França.

The main purpose of this work is to predict the peak interlaminar stress, responsible for the initiation of delamination, on a composite curved beam, subjected to end forces and end moments. The stacking sequence is symmetric, non-balanced, with 14 layers and it was fabricated using pre-impregnated unidirectional glass fiber in epoxy resin, stacked over a fabricated male tool, and the assembly was then vacuum-bagged and cured in a laboratorial autoclave. A sample of curved elements was tested to failure using static loads. Other sample was instrumented with strain gages in the outer and inner layers, in the apex region, and circumferential strains were measured. Two different finite element models were constructed in two commercial FEM applications: 1) 3D model with solid layered elements; 2) 2D model using plane elements. Interlaminar tensile and circumferential stresses obtained by FEM were compared. For the circumferential strains in the outer and inner layers, the results are validated with experimental data. The radial location and intensity of the interlaminar tensile stress were calculated by the Multilayer Theory of Ko and Jackson and were compared with the FEM results.

USING ASSESSMENT AS A TEACHING TOOL

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Based upon two personal beliefs, with regard to teaching that firstly "teaching is helping others to discover" and secondly that "assessment is a necessary inconvenience", a method has been developed in teaching Fluid Dynamics to undergraduate students, in a Mechanical Engineering Course. The main goal of this method is changing from a traditional theoretical approach of teaching "what is in the book" to a much more practical confrontation between theory and what can be found in laboratory experiment.
The program contents are covered by four laboratory apparatuses:
| Reynolds experiment,
| Head losses in tubes,
| Hydraulic turbines,
| Centrifugal pumps,
which are presented to all the students during a particular class so they can prepare for their next return to the laboratory, now organized into small groups. Meanwhile, each group must define their specific objectives and work planning, so the students can accomplish the experiments off-line, with the laboratory supervisor's eventual help and subsequent report must be written within a determined period. The main results achieved a success rate which has risen from about 50%, of the evaluated students before setting up the method to 70%, but keeping the same lecturer, i.e. the same quality demand.

Publicado em:
Proceedings of ASME IMECE 2006 2006 ASME International Mechanical Engineering Congress and Exposition November 5-10, 2006, Chicago, Illinois USA

CORROSION BEHAVIOUR OF NiTi ALLOY IN HANK'S SOLUTION

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Publicado em:
Livro de Resumos das Jornadas de Electroquímicas de Inovação 2006, p. 30, 20 de Outubro 2006, Porto, Portugal

Nitinol is a nickel-titanium nearly equiatomic alloy that has been attracting considerable interest for biomedical applications due to its shape memory and superelastic properties and biocompatibility. However, due to the high nickel content of the alloy and as this element may induce allergic response, the material should present superior corrosion resistance in contact with body fluids. Although several studies have been preformed on the corrosion performance of Nitinol when in contact with physiological media, there is a lack of reproducibility in the reported results and no information is available on the characterization of the material in dynamic conditions or after being deformed. In the present work, the electrochemical behaviour of NiTi has been studied in Hank's solution at 370C to simulate body conditions. The same study has been made on pure titanium and nickel in order to understand the contribution of each alloying element on the NiTi behaviour. It was observed that the corrosion behaviour of NiTi is much closer to Ti than to Ni, as may be seen on the polarization curve results, where the high protective character of the passive oxide film formed on NiTi is similar to that of titanium. The same conclusions were obtained using capacitance measurements (Mott-Shottky approach). An equivalent circuit was proposed to fit the impedance spectra of NiTi and electrochemical parameters were estimated to characterize its natural passive oxide film. XPS analysis established that both oxidized Ti and Ni can be found on the surface of polished NiTi alloy.

ELECTRODEPOSITION OF POLYANILINE ON ALUMINIUM ALLOY AA 6061-T6: ELECTROCHEMICAL ACTIVITY AND CORROSION PROTECTION PROPERTIES

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The use of pre-treatments on aluminium alloys prior to painting or adhesive bonding is an essential technology in many industrial sectors (e.g. aerospace industry). However, most of the pre-treatments currently used are based in chromates, which have been classified as hazardous to environment and human health. Thus, much effort has been undergoing to develop new coating systems. Since the publication of DeBerry's results on the corrosion protection properties of polyaniline on stainless steel [1], inherently conducting polymers (ICP) have been receiving increasing attention as possible components of corrosion-resistant coating alternative to chromate-based treatments. These polymers can be deposited on oxidisable electrodes by electropolymerization, which can simultaneously form and deposit polymer coatings on the substrate from a monomer-electrolyte solution. Among ICP's investigated for corrosion protection, polyaniline (PANI) has received the most attention. Nevertheless, the adhesion of the electrosynthesized PANI films is generally poor [2]. The present study covers the production of films of polyaniline on aluminium alloy AA 6061-T6 (used in aeronautical industry) by electropolimerization of aniline (0.5 M) in a solution 0.5 M H_2SO_4 and the investigation of their protective behaviour. The elctropolimerization was done making use of cyclic voltammetric or potentiostatic methods. Electrochemical activity and corrosion protection properties of the films were investigated by polarization curves, electrochemical impedance spectroscopy and cyclic voltammetry and compared with the electrochemical behaviour of the bare alloy.

Publicado em:
Livro de Resumos das Jornadas de Electroquímica e Inovação 2006, p. 23, 20 de Outubro 2006, Porto, Portugal

SUSCEPTIBILITY TO STRESS CORROSION CRACKING OF STAINLESS STEELS: THE ROLE OF MOLYBDENUM

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Publicado em:
Livro de Resumos do 57th Annual Meeting of the International Society of Electrochemistry, p. S9.O-23, 27 de Agosto a 1 de Setembro de 2006, Edimburgo, UK

The role of alloying elements on the susceptibility to Stress Corrosion Cracking (SCC) of stainless Steel is well documented in the literature, particularly the effect of molybdenum. However, the role of this element on film properties is not well understood. The approach used in this work includes the study of high purity austenitic Fe-Cr-Ni model alloys, with and without Mo additions, as well as the effect of deformation. A Mott-Schottky study was conducted complimented with polarization measurements in SCC environments containing chloride ions. Results show that Mo promotes stress corrosion cracking in the otherwise nonsusceptible alloy, confirming previous data. SCC is associated to the presence of a semiconducting film, which is predominantly p-type character (transport controlled by cationic vacancies). The doping density, estimated for samples with equivalent levels of plastic deformation was found to be larger for the Mo containing alloy. Mechanisms are discussed focussing the metal/film interface and the possible effect of dislocations on film properties, for the SCC case. The role of Mo regarding other types of localized corrosion such as pitting will also be discussed, on the basis of phenomena in the film/solution interface.

CORROSION BEHAVIOR OF NiTi ALLOY IN BODY FLUIDS

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In recent years NiTi shape memory alloys have attracted considerable interest for biomedical applications due to the combination of their mechanical properties (shape memory and superelasticity) and biocompatibility. However, due to the high nickel content of the alloy and as this element may induce allergic response, the material should present superior corrosion resistance in contact with body fluids. Although several studies have been preformed on the corrosion performance of Nitinol when in contact with physiological media, there is a lack of reproducibility in the reported results and no information is available on the characterization of the material in dynamic conditions or after being deformed. The present work deals with the preliminary results of a wide project aiming to understand the mechanisms of NiTi corrosion and to develop new surface treatments to enhance its corrosion resistance. The corrosion performance of Nitinol in human body simulating fluids was evaluated using polarization curves, open circuit potential measurements and electrochemical impedance spectroscopy at the body temperature (370C 0.50C).

Publicado em:
CD de Comunicações e Actas do Congresso Latino-Americano de Corrosão "LATINCORR 2006" p. 20, 21 a 26 de Maio 2006, Fortaleza, Brasil

FAULT DIAGNOSIS SYSTEM BASED IN AGENTS

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Publicado em:
Proceedings of the 6th IFAC symposium on fault detection, supervision and safety of technical processes (SAFEPROCESS'2006), Pequim, China, 29 Agosto – 01 Setembro de 2006.

ABSTRACT

In this work is proposed a new agent based fault diagnosis system for complex and dynamic processes. The fault diagnosis systems of the future should have present the distribution and complexity of the processes and they must be able to cooperate and communicate with other systems to achieve a satisfactory performance. The fault detection and isolation (FDI) agents proposed here have hybrid architectures based in a horizontal layered architecture. The reactive layer of the FDI agents are based in decomposition wavelet methods for the fault detection and in neural networks for the fault isolation task. The new agent based FDI system is applied to fault diagnosis in a three tank process.

FAULT DETECTION SCHEME USING THE AGENTS PARADIGM

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An agent based fault detection (FD) system for complex and dynamic processes is proposed in this work. The system is based in the agent paradigm where the modularity and complexity of the processes are important aspects in the FD system constructed. In the future, the FD agents must be able to cooperate and communicate with other systems to achieve a satisfactory performance, as a part of a fault tolerant control multi-agent system. The FD agents proposed here have hybrid architectures based in a horizontal layered architecture. Two types of FD agents are proposed, one based in decomposition wavelet methods with limit checking and other based in neural networks ARX models for residual generation. The agent based FD scheme proposed is applied in a three tank process.

Publicado em:
Proceedings of the 7th Portuguese Conference on Automatic Control (CONTROLO'2006), Lisboa, Portugal, 11-13 de Setembro de 2006.

FDI/FTC FOR COMPLEX NETWORKED CONTROL SYSTEMS BASED ON MULTI-AGENTS

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Publicado em:
Proceedings of the NeCST'06 - 2nd International Workshop on Networked Control Systems: Tolerant to Faults, Rende, Itália, 23-24 de Novembro de 2006.

When dealing with large-scale complex networked control systems, designing FDI/FTC systems is a very difficult task due to the large number of sensors and actuators spatially distributed and networked connected. Any solution given to this problem must take into account that practitioners prefer rather simplistic solutions since in practice, simple and verifiable principles always win the competition versus complex solutions that are usually characterized by instability, unpredictable behaviour and large computational burden. The FDI/FTC framework presented in this paper is able to achieve this goal by using simple and verifiable principles coming mainly from a decentralized design based on causal modelling partitioning of the NCS and distributed computing using multi-agents systems, allowing the use of well established FDI/FTC methodologies or new ones developed taking into account the NCS specificities.

AN ENGINE FOR LEAN IDEATION, PRODUCT CREATION & DEVELOPMENT

Gaspar, José Manuel Ferreira

Tese: (Mestrado em Engenharia de Concepção)
Orientadores: Arlindo Silva, Elsa Henriques
Instituto Superior Técnico, Fevereiro de 2007

RESUMO
Os mercados estão a preferir produtos novos com um tempo de entrega reduzido, exigindo assim, mais do processo de criação e desenvolvimento de produto. Mas o processo é disciplinado e usa etapas de decisão que não conseguem satisfazer as novas exigências. Como resultado a sua organização tem vindo a ser alterada de modo a ser mais flexível, adaptável e eficiente para acompanhar esta exigência, que está a aumentar depressa. Um dos aspectos essenciais do processo é o da criação e fluxo de informação. A maior parte desta informação é desperdício e o seu fluxo é descontínuo, criando assim, ineficiência e rigidez. Alguma pesquisa tem vindo a ser realizada de modo a aplicar a filosofia de emagrecimento ou de remoção de desperdício ao processo, principalmente no fluxo de informação – abordagem ao processo guiado por informação – mas não no seu âmago, isto é, a unidade de geração de informação ou motor de ideação. Assim o objectivo desta tese é o de propor um motor de ideação eficaz – ou magro – que cria informação útil e contribui para alterar efectivamente o processo. O requisito de fluxo contínuo foi integrado na nova estrutura conceptual de ideação, pelo uso de técnicas simples que reduzem a distracção da mente, isto é, que a mantém a operar num permanente fluxo consciente de informação. A nova estrutura conceptual foi validada por um caso de estudo desenvolvido no campo da engenharia de concepção.


04

ENGENHARIA QUÍMICA

Anuário Científico 2006

ISEL

RHENIUM COMPLEXES OF TRIS (PYRAZOLYL)METHANES AND SULFONATE DERIVATIVE

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The trioxo $[ReO_3\{SO_3C(pz)_3\}]$ (**1**) (pz = pyrazolyl) and oxo $[ReOCl\{SO_3C(pz)_3\}(PPh_3)]Cl$ (**2**) compounds with tris (pyrazolyl) methanesulfonate were obtained by treatment of Re_2O_7 or $[ReOCl_3(PPh_3)_2]$, respectively, with $Li[SO_3C(pz)_3]$, whereas $[ReCl_3\{HC(pz)_3\}]$ (**3**), $[ReCl_3\{HC(3,5\text{-}Me_2pz)_3\}]$ (**4**) and $[ReCl_4\{h^2\text{-}HC(pz)_3\}]$ (**5**) were prepared by reaction of $[ReOCl_3(PPh_3)_2]$ (**3,4**) or $[ReCl_4(NCMe)_2]$ (**5**) with hydrotris (pyrazolyl) methane $HC(pz)_3$ (**3,5**) or hydrotris (3,5-dimethyl-1-pyrazolyl) methane $HC(3,5\text{-}Me_2pz)_3$ (**4**). $[ReO\{SO_3C(pz)_3\}\{OC(CH_3)_2pz\}][ReO_4]$ **6**, with a chelated pyrazolyl-alkoxide, was derived from an unprecedented ketone-pyrazolyl coupling on reaction of crude **1** with acetone. The compounds have been characterized by elemental analyses, IR and NMR spectroscopies, FAB-MS spectrometry and cyclic voltammetry and, in the case of **5** and **6**, also by single crystal X-ray diffraction. The electrochemical *E*L Lever parameter has been estimated, for the first time, for the $SO_3C(pz)_3^-$ and oxo ligands allowing the measurement of their electron-donor character and comparison with other ligands. Compounds **1**, **2** and **6** appear to be the first tris (pyrazolyl) methanesulfonate complexes of rhenium to be reported.

Publicado em:
Dalton Trans., 2006, 4954-4961.

REDOX BEHAVIOUR OF A TRIS (PYRAZOLYL) METHANESULFONATE VANADIUM COMPLEX, A PRELIMINARY STUDY

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The electrochemical behaviour of the new vanadium(IV) complex $[VCl_3(SO_3Cpz_3)]$ (pz = pyrazolyl), obtained by reaction of VCl_3 with $Li[SO_3Cpz_3]$, investigated by cyclic voltammetry and controlled potential electrolysis is reported and compared with those of hydrotris (pyrazolyl) borate vanadium(IV) complexes.

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Portugaliae Electrochim. Acta., 2006, 24, 257-259

04

SYNTHESIS, CHARACTERISATION AND MOLECULAR HYPERPOLARISABILITIES OF PESUDO-OCTAHEDRAL NYDRIDENITRILEIRON(II) COMPLEXES FOR NONLINEAR OPTICS. X-RAY STRUCTURE OF [FE(H)(DPPE)$_2$(4-NCC$_6$H$_4$NO$_2$)][PF$_6$].CH$_2$CL$_2$

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A series of ionic pseudo-octahedral trans-hydridenitrileiron(II) complexes (general formula: [Fe(H)(dppe)$_2$(4-NCR)][PF$_6$], dppe = 1,2 bis (diphenylphosphino)ethane, R = structurally varied acceptor-substituted conjugated ligand), has been synthesised by chloride abstraction of the starting compound trans-[FeHCl(dppe)$_2$] and fully characterised. First hyperpolarisabilities β have been determined by hyper-Rayleigh scattering (HRS) at the fundamental wavelength of 1072 nm and the high near-resonant values obtained (up to 1130 x 10^{-30} esu) are interpreted in terms of the two-level model (TLM) and are correlated with IR and NMR spectroscopic data. Wavelength dependent HRS has been performed in the 1072 – 1580 nm range for two of the compounds [Fe(H)(dppe)$_2$(4- NC(CH)(CH)C$_6$H$_4$NO$_2$)][PF$_6$] and [Fe(H)(dppe)$_2$(4- NCC$_6$H$_4$(CH)(CH)C$_6$H$_4$NO$_2$)][PF$_6$]. These results clearly show the two-photon resonance but also the shortcomings of the TLM to derive reliable static b values. A structural study by X-ray diffraction of the compound [Fe(H)(dppe)$_2$(4-NCC$_6$H$_4$NO$_2$)][PF$_6$] shows crystallisation in the centrosymmetric monoclinic space group, P2$_1$/n, having four molecules in the unit cell with a pairwise antiparallel alignment of the dipoles.

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Eur. J. Inorg. Chem., 2006, 2175-2185

THE EFFECT OF COUNTER-IONS ON THE SUPRAMOLECULAR ARRANGEMENT OF (BENZONITRILE) [1,2-BIS(DIPHENYLPHOSPHINO)-ETHANE] (h5-CYCLOPENTADIENYLIRON(II) CATIONS

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Publicado em:
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The title compound [1,2-bis(diphenylphosphino)ethane](η⁵-cyclopentadienyl)(4-nitrobenzonitrile)iron(II) iodide, [Fe(η⁵-C_5H_5)($C_7H_4N_2O_2$)($C_{26}H_4P_2$)]I, crystallizes in the noncentrosymmetric space group *Cc*, which is a promising result for obtaining quadratic non-linear optical properties. However, the packing shows that the iodide counter-ion promotes the cancellation of almost all the dipoles, resulting in a supramolecular motif of cationic chains aligned in opposite directions making an angle of 35.2º. The use of the PF_6- as counter-ion induces the crystallization of the complex in a centrosymmetric space group. These results show that the introduction of different counter-ions, of different size and geometry, allows specific and directional intermolecular interactions that can determine the formation of a particular type of crystal packing.

SOLUBILITY OF METHANE IN WATER AND IN A MEDIUM FOR THE CULTIVATION OF METHANOTROPHS BACTERIA

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Solubility of methane in water and in an aqueous growth medium for the cultivation of methanotrophs bacteria was determined over the temperature range 293.15 to 323.15 K and at atmospheric pressure. The measurements were carried out in a Ben-Naim/Baer type apparatus with a precision of about ±0.3%. The experimental results were determined using accurate thermodynamic relations. The mole fractions of the dissolved gas at the gas partial pressure of 101.325 kPa, the Henry coefficients at the water vapour pressure and the Ostwald coefficients at infinite dilution were obtained. A comparison between the solubility of methane in water and those observed in fermentation medium over the temperature range of 298.15 to 308.15 K has shown that this gas is about ±2.3% more soluble in water.

The temperature dependence of the mole fractions of methane was also determined using the Clarke–Glew–Weiss equation and the thermodynamic quantities, Gibbs energy, enthalpy and entropy changes, associated with the dissolution process were calculated.

Furthermore, the experimental Henry coefficients for methane in water are compared with those calculated by the scaled particle theory. The estimated Henry coefficients are about ±4% lower than the experimental ones.

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Journal of Chemical Thermodynamics, 2006, vol. 38, 1629-1633

AVALIAÇÃO DE COMPOSTOS FENÓLICOS E FLAVONÓIDES EM MEL DE DIFERENTES REGIÕES DE PORTUGAL

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A importância da pesquisa de compostos fenólicos e flavonóides em alimentos deve-se ao facto de muitos destes compostos apresentarem propriedades antioxidantes.

A acção dos antioxidantes no combate ao stress oxidativo tem sido objecto de estudo em diversos trabalhos que demonstram a importância destes compostos na prevenção de doenças associadas ao envelhecimento, diminuindo o risco de doenças cardiovasculares e o aparecimento de cancro.

Sendo o mel um produto natural, tradicionalmente utilizado em Portugal, a avaliação da sua capacidade antioxidante poderá conduzir a uma valorização do produto junto do consumidor. Com efeito, estudos recentes mostraram a existência de fenóis e flavonóides no mel de outros países que, juntamente com a prolina, contribuem para a actividade antioxidante deste produto.

O objectivo deste trabalho foi a determinação do teor em compostos fenólicos totais e flavonóides em mel de diversas regiões de Portugal com origem mono e multifloral, constituindo estes estudos um ponto de partida para a avaliação da capacidade antioxidante do mel de produção nacional.

A quantificação destes compostos foi realizada através de espectrometria de absorção molecular na zona do visível. Na determinação dos compostos fenólicos totais foi usado o método de Folin-Ciocalteu e na quantificação dos flavonóides foi aplicado o método de Dowd com as modificações sugeridas por Meda et al.

Os resultados permitiram estabelecer comparações entre os méis das diferentes regiões e especular sobre a possível influência da flora local no teor dos compostos em estudo.

THE CORROSION RESISTANCE OF HOT DIP GALVANISED STEEL AND AA2024-T3 PRE-TREATED WITH BIS-[TRIETHOXYSILYLPROPYL] TETRASULFIDE SOLUTIONS DOPED WITH $CE(NO_3)_3$

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The present work aims at evaluating the anti-corrosion behaviour of a novel pre-treatment based on bis-[triethoxysilylpropyl] tetrasulWde (BTESPT) doped with cerium nitrate for application on hot dip galvanised steel and AA2024-T3 substrates. The corrosion resistance was evaluated by electrochemical impedance spectroscopy (EIS) and by the scanning vibrating electrode technique (SVET), during immersion in NaCl solutions. The electrochemical results showed that the pre-treatment provides excellent corrosion protection to the subs-trates. Furthermore, the results evidenced improved protection comparatively to the use of undoped BTESPT pre-treatments, both for galvanised steel and AA2024-T3. This improvement is most likely due to enhanced barrier properties of the Wlm and additional active corrosion protection originated from the inhibiting action of the cerium-based inhibitor impregnated in the silane matrix.

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Corrosion Science, 48 (2006) 3740-3758

THE CORROSION RESISTANCE OF HOT DIP GALVANISED STEEL PRE-TREATED WITH BIS-FUNCTIONAL SILANES MODIFIED WITH MICROSILICA

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Publicado em:
Surface Coatings Technology, 200 (2006) 2875-2885

The present work aims at understanding the corrosion behaviour of hot dip galvanized steel pretreated with either bis-1,2-[triethoxysilyl] ethane silane (BTSE) or bis-[triethoxysilylpropyl] tetrasulfide (BTESPT) modified with microparticles of SiO_2. The corrosion resistance was evaluated by electrochemical impedance spectroscopy, potentiodynamic polarization and by the scanning vibrational electrode technique (SVET) during immersion in dilute NaCl solutions. The films formed on the galvanized steel substrate were characterized by X-ray photoelectron spectroscopy, Auger electron spectroscopy and atomic force microscopy. The results show that the pretreatments based on silane films modified with silica particles provide corrosion protection for hot dip galvanized steel during immersion in NaCl-containing solutions.

INFLUENCE OF THE DEPOSITION PARAMETERS ON THE PROPERTIES OF BIS-[TRIETHOXYSILYLPROPYL] TETRASULFIDE (BTESPT) LAYERS ON AA2024-T3 – AN ELLIPSOMETRIC STUDY

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A bis-sulphur silane (BTESPT) was used to produce thin protective layers on AA2024-T3, a structural aluminium alloy widely used in the aeronautic industry, being the coatings analysed ex-situ by ellipsometry. Despite a slight degree of film anisotropy evidenced by measurements at different angles of incidence, an optical model of a single homogeneous phase could be employed to describe the silane based layer. The information obtained allowed to characterize the influence of the operational deposition parameters on the film thickness and structural organization of the silane phase (evaluated by its optical absorption). It is shown that the silane concentration of the solution and immersion time determine the final thickness of the formed layer while the curing time does not affect significantly this parameter. On the other hand, it was observed a marked decrease of the optical absorption of the coatings submitted to curing temperatures of at least 100ºC, which should be ascribed to a structural reorganization phenomena induced by the removal of water molecules from the film. The data gathered by ellipsometry were successfully corroborated by independent surface profilometry analysis of the films.

Publicado em:
Materials Science Forum, 514-516 (2006) 682

FOREST FIRES IN PORTUGAL: HOW IT HAPPENED AND WHY IT HAPPENED

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Publicado em:
International Journal of Environmental Studies, 2006, 63(2), 109 - 119

Forest fires are recurrent phenomena in Southern European countries, due to the nature of Mediterranean forest and climatic characteristics. In Portugal, however, in the recent years, forest fires have become a public calamity and are now endangering the sustainability of the forest itself, as well as several derived economic activities. This paper reviews the past and current situation of forest fires in Portugal, analyses its main causes and consequences and derives recommendations to overcome this problem.

"FUME EMISSIONS DURING GAS METAL ARC WELDING"

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The control of exposure to welding fumes is of increasing importance in promoting a healthy, safe and productive work environment. This article describes the effects of shielding gas composition on the amount and composition of welding fumes produced during gas metal arc welding (GMAW). The amount of fumes generated during welding was measured for steady current over a range of wire-feed speeds and arc voltages of using the standard procedures contained in ANSI/AWS F1.2. Results of these measurements show that the fume formation rates (FFRs) increase with CO_2 and O_2 in the shielding gas mixture. The lowest FFRs were obtained with the mixtures of Ar+2%CO_2 and Ar+3%CO_2+1%O_2. The highest FFRs were obtained with the mixtures Ar+18%CO_2 and Ar+5%CO_2+4%O_2. The welding fume contains mainly iron, manganese, silicon, titanium and sodium under oxide forms. The fume cluster particles have dimensions between 0.5 and 2 μm. The FFR was found to be governed by the transfer modes of molten metal, i.e. the current intensity and arc voltage, as well as by shielding gas mixtures composition. Thus these parameters have to be taken into consideration before designing a welding process. Whenever possible, users of GMAW should use the lowest current intensity. However, when this is not possible, due to the constraints of process productivity, welders should use higher currents, but with Ar+2%CO_2 and Ar+3%CO_2+1%O_2 shielding mixtures, which will lead to smaller fume emissions.

Publicado em:
Toxicological and Environmental Chemistry, 2006, 88(3), 385 - 394

"ESTIMATION OF UNCERTAINTY IN THE DETERMINATION OF NITROGEN OXIDES EMISSIONS"

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Publicado em:
Accreditation and Quality Journal, 2006, 11(3), 138 – 145

This paper presents a methodology for estimation of uncertainty on a reference test method for determination of nitrogen oxides concentration in gaseous emissions from stationary sources. As a first stage for identification of uncertainty sources, the test method is carefully reviewed in detail. Afterwards, these sources are quantified, bearing in mind its partial uncertainty, allowing the determination of the combined uncertainty and, finally, the expanded uncertainty. The calculation procedure was implemented into an excel calculation file. Using this file and considering several numerical applications from real situations, uncertainities around 15 mg/Nm^3 over determined concentrations of 350 mg/Nm^3 of NOx (expressed as NO_2) were obtained.

"LEACHING OF HEAVY METALS FROM STEELMAKING SLAGS"

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Leaching tests with EAF and Ladle slags were performed, using a flow through test and the standard batch test DIN 38414-S4. The previous method was used to simulate the leaching behaviour of steel slags under landfill. The chemical analysis of the leachates during this period shows, in general, for both types of slag, an increase of heavy metal releases with ageing. Standard test method DIN 38414-S4 was used to evaluate leachability of heavy metals by water in unprocessed slags. After more than one year of trials, slag samples submitted to these trials presented very low total leaching levels. The most extracted elements are calcium and magnesium. Nevertheless, in flow-through test, calcium and magnesium leached from solid slags are below 0.5% and all other metals below 0.1%. Leachates obtained with DIN 38414-S4 present, as expected, higher leaching values; however, these are inferior to 5% (Ca) and 1% (other elements).

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Revista Metalurgia Madrid, 2006, 42(6), 409 – 416

04

"CORK PROCESSING WASTEWATERS TREATMENT BY AN OZONIZATION/ ULTRAFILTRATION INTEGRATED PROCESS"

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Publicado em:
Desalination, 2006, 191, 148 – 152

Membrane fouling has been identified as one of the major problems during the treatment by ultrafiltration (UF) of the cork processing wastewaters. This problem leads to the drastic reduction of the UF permeate fluxes and is often attributed to the fact that these wastewaters are rich in phenolic/tannic colloidal matter. In order to understand and minimize membrane fouling, this work addresses a systematic evaluation of the ultrafiltration of cork processing wastewaters, in terms of UF membrane characteristics, UF operating conditions and consideration of an integrated process of ozonization/ultrafiltration. The goal for the ozonization pre-treatment is to reduce the phenolic/tannic colloidal matter content and correlate that with the membrane fouling and the UF permeate fluxes enhancement.

Five ultrafiltration membranes were investigated: a commercial membrane, TS60 (Ropur) and four laboratory made cellulose acetate membranes. They cover a wide range of molecular weight cut-offs, from 4 to 98 kDa. The ultrafiltration experiments are carried out in flat-sheet cells of 13.2 cm^2 of membrane surface. The UF operating conditions are varied in terms of the hydrodynamics, circulating velocities of 100 l/h and 200 l/h, and in terms of transmembrane pressures, from 1 to 3 bar. The ozone pre-treatment led to a reduction of 11% in the total organic carbon content and to a reduction of 51% in the total polyphenols content, these reductions led to the enhancement of the UF permeate fluxes.

"OPTIMIZATION OF SACCHARIDE FRACTIONATION USING NANOFILTRATION/ULTRAFILTRATION"

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Galacto-oligosaccharides (GOS) have limited digestibility, prebiotic properties and low-calorie sweetener potential. Therefore, are dietary food ingredients with a significant world annual production (over 15,000 t/yr). GOS are produced from the lactose — present in second cheese whey — using enzyme reactors (with b-galactosidases). Short residence times in a continuous bioreactor allow higher GOS concentration in the outflow, unfortunately together with the unreacted substrate. This means that to obtain a better industrial product it is very important to develop processes able to fractionate such a stream in mono-/di- and tri-/oligosaccharides. Then, unreacted lactose could be recycled to the enzyme reactor. Nanofiltration (NF) has a high potential for industrial application in a GOS production process as it is reliable and simple to scale-up. The fractionation of saccharides and oligosaccharides by nanofiltration depends on: membrane pore size distribution [1], solutes concentration and pH. This work investigates the dependence of the fractionation of low molecular weight model-saccharide mixtures on the membrane molecular weight cut-off (MWCO) and on the solute concentration. The model saccharides tested were glucose, sucrose, lactose, raffinose and melezitose.

Publicado em:
Desalination, 2006, 199, 337 – 339

"EM QUE PONTO ESTAMOS RELATIVAMENTE À CAMADA DE OZONO?"

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Publicado em:
Ingenium, 2006, 91, 94

O "buraco" da camada de ozono tem sido considerado como uma história de sucesso das políticas ambientais globais, tanto mais que se verificou, recentemente, que pela primeira vez nos últimos 50 a 100 anos a abundância de substâncias que provocam a depleção do ozono na atmosfera (SDO) na atmosfera entrou em declínio. Com efeito, cerca de dois anos após a sua descoberta, sobre a atmosfera da Antárctica, os governos de diversos países, entre os quais a maioria dos países da União Europeia, assinaram em 1987 um acordo, chamado Protocolo de Montréal, com o objectivo de reconstituir a concentração de ozono na alta atmosfera. Este acordo entrou em vigor em 1989 e visa reduzir, progressivamente, as emissões dos gases que provocam a deplecção do ozono, tais como os CFC (cloro-fluoro-carbonados), presentes nos fluidos frigoríficos, gases propulsores e agentes extintores e retardantes de chama. Uma vez que os CFC têm um tempo de vida média na atmosfera compreendido entre 50 e 100 anos, os gases que entretanto foram emitidos, vão continuar a fazer a sua acção destruidora durante muito tempo. Além disto, a destruição do ozono na alta atmosfera ocorre, em maior extensão, quando a temperatura destas camadas é baixa. Nestas condições, este efeito conhece variações sazonais. Com efeito, no ano 2000, as dimensões do "buraco" da camada de ozono atingiram um valor máximo de 27 a 28 milhões de km^2, devido a um Inverno particularmente frio. Em 2002, as dimensões sofreram um decréscimo e o "buraco" foi mesmo dividido em duas partes distintas, devido a uma vaga de calor sem precedentes na região.

Tudo isto nos leva a crer que, enquanto anteriormente se pensava que este fenómeno era totalmente independente das emissões dos gases de estufa, tais como o dióxido de carbono; os dois fenómenos podem, de facto, estar relacionados. Isto porque o aquecimento climático é acompanhado de um arrefecimento da alta atmosfera em altitude, o que pode acelerar a destruição da camada de ozono. Anteriormente à descoberta da possível correlação entre estes dois fenómenos estimava-se que a recuperação da camada de ozono não deveria começar a ocorrer antes de 2010-15, e que a recuperação com-

pleta dessa mesma camada só poderia começar a ser esperada cerca de 2050-60. A eventual correlação entre os dois fenómenos poderá resultar na revisão, para mais longe, destas expectativas, a menos que o Protocolo de Kyoto venha a ter resultados positivos em breve, sobre a diminuição das emissões de gases com efeito de estufa.

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

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

CALIX[n]ARENE-PS-DVB (n=4,6,8) AND β-NAPHTOL: HOST-GUEST INTERACTIONS IN AQUEOUS MEDIA

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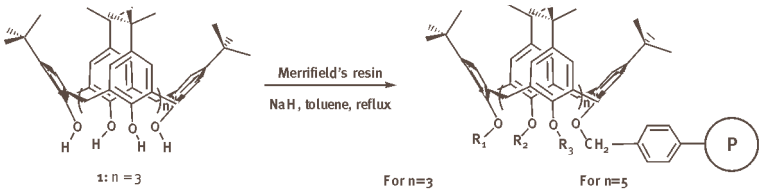
When a molecule or a supramolecule uses its concave surfaces (cavities) as binding sites, the host (receptor) may be able to recognize a guest (substrate) on a structural complementarity basis. In the field of calixarene chemistry, this concept was nicely illustrated with the pioneering work of Gutsche and his co-workers on the complexation of aromatic hydrocarbons by water-soluble calix[h]arenes (n=4,6,8).



1: n = 3
2: n = 5

For n=3
3: $R_1=R_2=R_3=H$;
5: $R_1=R_2=H$; $R_3=CH_2CO_2Et$;
7: $R_1=R_2=H$; $R_3=CH_2CO_2H$;
9: $R_1=R_2=H$; $R_3=CH_2CO_2Na$;

For n=5
4: $R_1=R_2=R_3=H$
6: $R_1=H$; $R_2=R_3=CH_2CO_2Et$
8: $R_1=H$; $R_2=R_3=CH_2CO_2H$
10: $R_1=H$; $R_2=R_3=CH_2CO_2Na$

Scheme 1. **3** or **4**, $BrCH_2CO_2Et$, K_2CO_3, acetone, reflux ⟶ **5** or **6**; **5** or **6**, NaOH aq., THF, reflux, acidic *w-up* ⟶ **7** or **8**; **7** or **8**, NaOH aq. 10%, THF, r.t. ⟶ **9** or **10** (for compounds **5-10**, the specific location of the substituents in the lower rim was not determined).

It is know that a number of factors affects the strength of binding of neutral organic molecules by calixarene receptors, namely the type of interaction, nature of the guest, preorganization of the host and solvation effects. The majority of these studies focuses on the recognition abilities of conformational rigid calix[4]arenes on apolar media or in the solid state. Complexation with these types of hosts is, however, restricted to small organic molecules (*eg.* CH_3CN, CH_3NO_2, $(CH_3)_2CO$, $C_6H_5CH_3$) due to the limited molecular dimensions of the internal cavity of the host. We have been interested in the last few years in the synthesis of calixarene-based polymers and, in general, materials containing calixarene units along a polymeric chain, owing to their potential usefulness in several areas of host-guest and sensing chemistry.

In this communication we report on the synthesis and characterization of polymer-bound calix[n]arenes (n=6,8), based on our previously described protocol for the tetramer analog, which involve the direct attachment of the appropriate *p-tert*-butylcalix[n]arene in its hydroxyl form to a Merrifield type resin, a lightly cross-linked polystyrene-divinylbenzene (PS-DVB), with further modification of the resultant polymers by the introduction of hydrophilic groups in the calixarene unit (Scheme 1). Using β-naphtol (BN, a common azo dye coupling component) as a model guest, the sorption abilities of the thus formed calix[n]arene-PS-DVB was next examined. The solid-liquid extraction of the pollutant (BN) from aqueous solutions (0.75 mM) was performed under batch conditions. The results clearly revealed that the dimensions of the cavity of the grafted calixarene unit is of utmost importance for the success of BN sorption (calix[8]›calix[6]››calix[4]), as well as the extent of hydrophilic character of the substituents on the lower rim of the calixarene unit (-CO_2^-››-CO_2H››-OH).

NOVEL CONJUGATED CALIX[4] ARENE-BASED POLYMERS: Rh(I) CATALYZED POLYMERIZATION OF SYN-DISTAL-DIPHENYLETHYNYL-CALIX[4]ARENE COMPOUNDS

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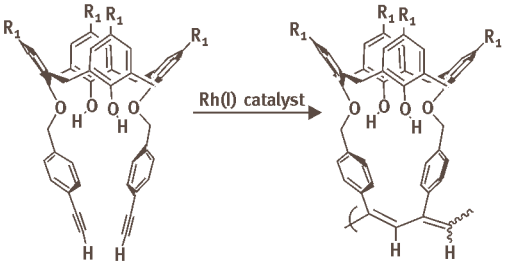
Conjugated polymers incorporating macrocyclic receptors within their structure, either as pendant groups or as part of a polymeric backbone, inasmuch as they may combine the electroconductive, magnetic and optical properties of the conjugated polymer backbone with the ability of the macrocyclic units to perform host-guest chemistry, are very interesting and useful molecular materials, owing to their potential uses in sensing chemistry (*eg.* as electrochemical switches, electronic and optoelectronic devices and sensors). In these systems, the chemical sensing relies in specific and non-specific analyte-receptor interactions transduced into a measurable response, normally evaluated with conductometric, potentiometric, colorimetric or fluorescence methods. Crown and aza-crown ethers, cyclodextrins and calixarenes, tethered through a spacer to chemical or electro polymerizable moieties such as thiophenes, pyrroles or phenylacetylenes, are representative examples of these systems.



1: R_1 = *t*-butyl
2: R_1 = H

poly 1: R_1 = *t*-butyl
poly 2: R_1 = H

In this communication we report on our latest work regarding the synthesis and characterization of novel conjugated polymers having a calix[4]arene receptor incorporated into the main chain, following a cyclo-polymerization route previously explored by us on divinylbenzyl-calix[4]arene derivatives. Appropriate calix[4]arene derivatives were successfully functionalized in the lower rim via an improved Sonogashira-Hagihara cross-coupling procedure, affording the *syn*-distal-

diphenylethynyl-calix[4]arene compounds **1** and **2** (see accompanying communication on this subject). The ability of these building blocks to behave as bifunctional monomers toward the synthesis of conjugated polymers was next evaluated. It was found that Rh(I) catalyzed polymerization of **1**, having triphenylphosphine as the solely additive (2 mol% $[Rh(nbd)Cl]_2$; $[Rh]:[PPh_3]=0.5$), smoothly produce the expected conjugated polymer poly **1** in good yield. For the debutylated homolog **2**, its polymerization was best carried out in the absence of any added co-catalyst. The linear nature of poly **1**, which showed number-average molecular weights up to $1.1x10^5$ $gmol^{-1}$ and low polydispersities, was deduced from the collected spectroscopic data (FT-IR, ^1H NMR, ^{13}C NMR and UV-vis), the unimodal pattern of the GPC profiles and their solubility in common nonprotic organic solvents. A highly selective ring-closing polymerization of **1** and **2**, through an alternating intra-intermolecular chain mechanism, is proposed to explain the polymerization results.

AN EFFICIENT SYNTHESIS OF SYN-1,3-DIPHENYLYNE-CALIX[4]ARENE COMPOUNDS USING AN IMPROVED SONOGASHIRA CROSS-COUPLING PROTOCOL

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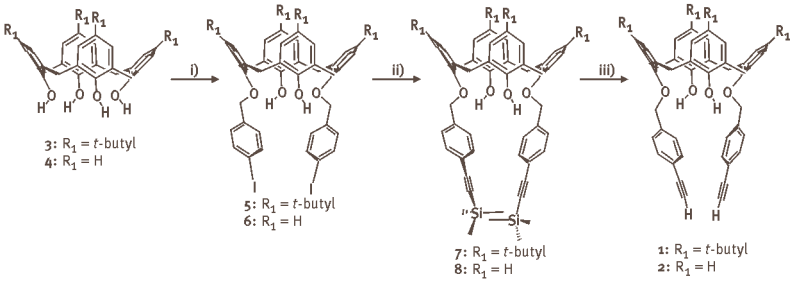
Publicado em:
Livro de Resumos do XX Encontro Nacional da Sociedade Portuguesa de Química, Monte da Caparica, Portugal, 2006.

As part of our ongoing research regarding the synthesis of conjugated calixarene-based polymers (see accompanying communication on this subject), there was a need to develop an adequate synthetic route towards the *syn*-1,3-bis(4-ethynylbenzyloxy)calix[4]arenes **1** and **2**. The envisage strategy is outlined in Scheme 1. Selective derivatization of the parent *p*-R_1-calix[4]arenes **3** and **4** with 4-iodobenzyl bromide in acetonitrile, using either K_2CO_3 or Na_2CO_3 as base, afforded the intermediate diiodo compounds **5** and **6**, respectively, in good yields. The subsequent diethynylation of **5** and **6** was performed under conditions of the Sonogashira-Hagihara cross-coupling protocol.



Scheme 1. Synthesis of calix[4]arenes **1** and **2**: i) $BrCH_2PhI$, K_2CO_3, CH_3CN, reflux, 24h; ii) $PdCl_2[PPh_3]_2$, CuI, $(CH_3)_3SiC{\equiv}CH$, PPh_3, THF and $NHEt_2$, 120ºC, 0.75h; iii) (*n*-Butyl)$_4$NF, THF, 25ºC, 0.5h.

In our preliminary work, the ethynylation of **5** was carried out with either $Pd(OAc)_2$ or $PdCl_2[PPh_3]_2$ as catalysts (2.5 mol%), copper iodide (1.5-5 mol%) as co-catalyst and NEt_3 (THF used as co-solvent) or piperidine as base, using trimethylsilylacetylene (TMSA) as ethynylation reagent. These initial experiments showed that, after 24h at 50ºC, the desired product **7** was obtained in 66% yield, along with *ca.* 5% of the monoethynyl derivative, when NEt_3/THF were used in conjunction with $Pd(OAc)_2$. The use of piperidine as base proved to be the worst choice, whatever the catalyst used, resulting in much less clean reactions under the same experimental conditions, show-

ing, besides **7**, *ca.* 40% of the monocoupled product when $Pd(OAc)_2$ was used; the outcome was even worse with $PdCl_2[PPh_3]_2$. A remarkable improvement was achieved for the coupling reaction when the diiodo compounds **5** and **6** were coupled with TMSA at 120ºC in THF in a closed vessel, using $PdCl_2[PPh_3]_2$ as the Pd(0) source, CuI as co-catalyst and $NHEt_2$ as base. Under otherwise identical stoichiometric relationships to those previously tested, a very clean and complete reaction occurs within 0.5-1h, affording the protected diethynyl compounds **7** and **8**, respectively, in very good to excellent isolated yields. The NMR data of the resulting bis-trimethylsilylethynyl derivatives **7** and **8** evidences the presence of C_{2v}-symmetrical structures in the cone conformation. Deprotection of the ethynyl groups with $(n\text{-butyl})_4NF$ in THF (0.5h, 25ºC) afforded compounds **1** and **2** in fair to good isolated yields.

RING-CLOSING POLYMERIZATION OF 1,3-BIS-(4-ETHYNYLBENZYLOXY)-p-TERT-BUTYLCALIX[4]ARENE PROMOTED BY Rh(I) CATALYST

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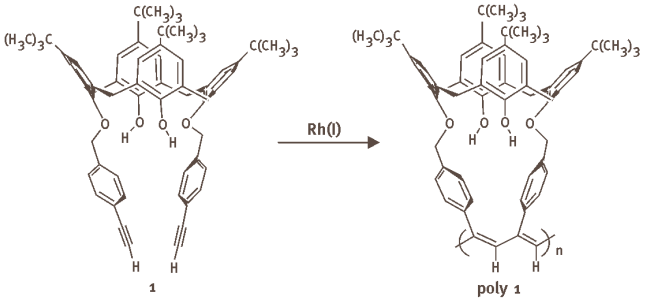
Conjugated polymers incorporating macrocyclic receptors within their structure are well-suited to perform sensing chemistry. Examples of these systems involving calixarenes, cyclodextrins and crown and azocrownethers are known. Recently, the radical cyclopolymerization of a divinylbenzyl-*p-tert*-butylcalix[4]arene derivative was accomplished. Here we report, for the first time, the synthesis of a conjugated calix[4]arene-based polymer (**poly 1**), in which the macrocycle is part of the main chain. It is expected that with this polymer architecture, the host-guest interactions could be efficiently transduced into a measurable response through the intermediacy of the polyene chain.

The ethynyl functionalities on the lower rim of the starting monomer **1** were introduced via a Sonogashira-Hagihara cross-coupling reaction in a three-step sequence from the parent calix[4]arene.

Polymerization of **1** using a Rh(I) catalyst was studied under a variety of conditions. Solvent effects were found in the Mn of the resultant polymers but not in their polydispersity. The effects of added co-catalysts ($NHEt_2$ and PPh_3) were also examined.

It was found that when **1** was polymerized in THF using 2 mol% of $[Rh(nbd)Cl]_2$ and triphenylphosphine as an additive ($[PPh_3]$:[Rh]=2), a high conversion was achieved (92%). Under these conditions and within 9h of reaction, a soluble material was isolated in good yield (74%).

The FT-IR, NMR and UV-Vis spectra of **poly 1**, in conjunction with GPC and solubility data, furnished evidence about its structure and unequivocally showed its conjugated nature.



Scheme 1. Cyclopolymerization of calix[4] arene 1

VOLTAMMETRIC ANALYSIS OF α-TOCOPHEROL IN VEGETABLE OILS

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Vitamin E represents a group of natural antioxidants which includes several tocopherol and tocotrienol compounds. The α-tocopherol, traditionally recognized as the most active form of vitamin E in humans, is a powerful biological antioxidant and an effective radical scavenger, protecting against the free radical attack. This important role is confirmed by recent research, suggesting that vitamin E deficiency is associated with an elevated risk of coronary heart disease and other degenerative process. Tocopherols are presented in vegetable oils and are responsible for many of the healthful properties of these food products. Furthermore, the determination of the tocopherols content in vegetable oils is very important in ascertaining the oils' durability as well as the stability of these products. The purpose of this work is the voltammetric analysis of α–tocopherol in several vegetable oils, namely, corn, sunflower, soyabean, peanut and wheatgerm. In this study, the differential pulse voltammetry (DPV) technique was used and the concentration of α–tocopherol was determined by the standard addition method.

The experiments were performed using a computer-controlled potentiostat mAutolab Type III, equipped with an IME663 interface and a Metrohm 663 VA stand, which included a single compartment three-electrode cell. The working electrode was a rotating disc electrode with glassy carbon electrode tip (GC-RDE). The reference electrode was an Ag/AgCl, LiCl saturated in ethanol and the counter electrode was a platinum rod. The DPV voltammograms were recorded between 0.550 V and 0.900 V with a scan rate of 10 mV/s and pulse amplitude of 50 mV. The anodic peak potential of α–tocopherol was found at about 0.688 V for all the vegetable oils. A separated voltammetric peak was also obtained for δ-tocopherol in soyabean oil at about 0.890 V. However, it was found that for the corn, soyabean, peanut and wheatgerm oils, the peaks of γ and β-tocopherols overlap at 0.800 V.

The accuracy of the method was verified by means of recovery assays, ranging the α–tocopherol recovery in the sunflower oil from 96.2 to 108.6%. Moreover, the α-tocopherol contents found in the vegetable oils samples are in the range of other literature data and in agreement with the concentration value of the package label.

APLICAÇÃO DE ULTRASSONS A AMOSTRAS DE MEL PARA ANÁLISE DE METAIS POR FAAS

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A determinação de metais em amostras de produtos alimentares é frequentemente realizada por espectrometria de absorção atómica com chama ou câmara de grafite. No entanto, a aplicação destes métodos requer, normalmente, um pré tratamento das amostras de modo a destruir matéria orgânica que possa interferir na análise.
Como as metodologias clássicas de pré tratamento são geralmente muito morosas, têm sido desenvolvidas e aplicadas novas técnicas entre as quais se destaca o uso de ultrassons.
O objectivo do presente trabalho foi o estudo da aplicação de ultrassons a amostras de mel nacional de origem monofloral e multifloral, analisando a influência de parâmetros como a massa de amostra, a composição da solução do ácido, o tempo e a amplitude de sonicação no doseamento do potássio por espectrometria de absorção atómica com chama. O teor em potássio determinado nas amostras de mel tratadas com ultrassons revelou uma boa concordância com o encontrado no mesmo tipo de amostras previamente tratadas por gravimetria.

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Livro de Resumos do XX Encontro Nacional da SPQ – Química Sustentável, Campus da Caparica, Portugal, Dezembro de 2006

APLICAÇÃO DO MODELO UNIFAC A SISTEMAS GÁS-LÍQUIDO

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Publicado em:
Livro de Resumos do XX Encontro Nacional da SPQ – Química Sustentável, Campus da Caparica, Portugal, Dezembro de 2006

Modelos de previsão e correlação de solubilidade de gases em líquidos desempenham um papel importante em Engenharia Química em virtude de ser impossível medir a solubilidade num amplo intervalo de pressão e temperatura para todos os sistemas gás-líquido.

Os métodos de contribuição de grupos, utilizados com frequência na previsão de propriedades associadas ao equilíbrio termodinâmico, têm sido recentemente aplicados a sistemas gás-líquido no sentido de prever e correlacionar os valores de solubilidade.

Neste trabalho é desenvolvida a metodologia a seguir na aplicação do modelo UNIFAC a sistemas gás-líquido e são apresentados os resultados obtidos na correlação dos valores de solubilidade de árgon e de metano em água, no intervalo de temperatura de 293,15 a 323,15K e à pressão atmosférica.

O uso do modelo UNIFAC, como método de correlação, permitiu a determinação dos parâmetros de interacção entre os grupos estruturais dos sistemas árgon-água e metano-água. O conhecimento destes parâmetros possibilitou, por sua vez, o cálculo dos valores de fracção molar de gás dissolvido, os quais apresentaram uma excelente concordância com os determinados experimentalmente.

PRODUCT CHARACTERIZATION OF CORIOLUS VERSICOLOR BIOMASS AS IMMUNONUTRIENT

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Publicado em:
First Annual Monro Medical Lecture at Royal College of Surgeons, London, U.K. 23rd September 2006. (lecture)

In addition to nutritional value, several mushroom strains have been used in traditional oriental therapies. In fact, a variety of species of mushrooms have shown medicinal effects such as blood pressure and cholesterol lowering, liver protection, anti-fibrotic, anti-inflammatory, anti-diabetic and anti-viral activities. Among these bio-pharmacological features, medicinal mushroom research has been focused on new features such as (products) with antitumour and immunostimulating pro-perties. For instance, a wide variety of protein-bound polysaccharides such as PSK (Polysaccharide Krestin) and PSP, both derived from *Coriolus versicolor*, act as immunomodulators or biological response modifiers. Both protein-bound polysaccharides PSK and PSP isolated (marketed in Japan and in Hong Kong respectively) are the best known commercial protein-bound polysaccharides which exhibit a wide range of biological response. These extremely important compounds have similar physiological activities but are structurally different. In fact, both products have a molar mass of about 100 kDa, their polypeptides contain large amounts of aspartic acid and glutamic acid, although PSP contains arabinose and rhamnose instead of fucose present in PSK. PSK is widely prescribed as adjuvant nutrition during chemotherapy and radiotherapy in Japan, while PSP has been extensively studied by Chinese scientists and also prescribed as an adjuvant by oncologists. The intake of these mushroom compounds improves the defence mechanisms, which restore homeostasis and homeorhesis, enhancing resistance to tumour induction, showing little evidence of side effects when taken with conventional cancer therapies as chemotherapy or radiotherapy. However, molecular mechanisms of biological response modification are not completely understood, although PSK and PSP are potent immunomodulators with specific activity for T-cells and for antigen-presenting cells such as monocytes and macrophages.

However, a recent report has been published which presents evidence about the presence of specific receptors for protein-bound polysaccharides in antigen-presenting cells (APC), B-cells and Helper T-cells. The binding of these complexes to these cells triggers a variety of

immunological responses such as modulation of immunoglobulin production, TH- cell differentiation and function and APC - TH interaction. On the other hand, several reports have been published about the induction of apoptosis of several human cancer cell lines due to binding of protein-bound polysaccharides from mushroom strains.
Pharmacologically active polysacchacarides and protein-bound polysaccharides can be isolated from mushrooms fruit-bodies, culture mycelium or culture broth of several basidiomycete strains such as *Coriolus versicolor*. Besides protein-bound polysaccharides, *Coriolus versicolor* contains several other biomolecules of clinical importance such as enzymes and secondary metabolites (e.g. antibiotics and terpenes).

CATALYTIC COMBUSTION OF TOLUENE ON COPPER EXCHANGED MFI AND Y ZEOLITES. EFFECT OF ADDITION OF CESIUM AND VANADIUM

Silva, Elisabete R.[1]; Batalha, Nuno[1]; Bartolomeu, Rui[1]; Silva, João M.[2]; Ribeiro, Fernando R.[1]; Ribeiro, Filipa[1]

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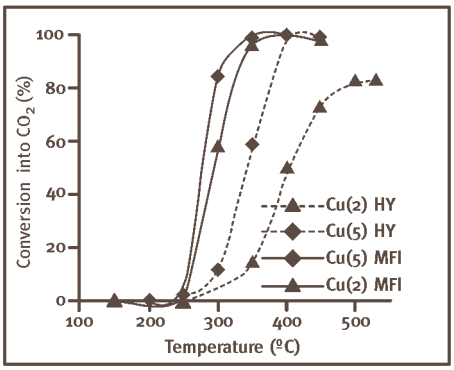
Publicado em:
XX Encontro Nacional da Sociedade Portuguesa de Química, FCT-UNL, Dezembro 2006

Volatile Organic Compounds (VOCs) are one of the main atmospheric pollutants, since they are indirectly associated to the increase of ozone [1]. New environmental legislation has established stringent regulations to control VOC emissions, as the Gotemburgo Protocole and the EU Council Directive 2001/81/EC. Catalytic oxidation has been identified as one of the most important and promising processes to destroy VOCs at low concentration. Catalysts based on supported noble metals are very efficient for VOCs combustion, but they are relatively expensive. From the activity point of view, copper supported on different materials, namely on zeolites, have been suggested as potential catalysts and as an alternative to noble metals [2]. In this work, CuHY and CuHMFI zeolites with copper (1-5 wt.%) or with copper and vanadium (5 wt.%) or cesium (5 wt.%) have been studied in catalytic combustion of toluene (800 ppm) with air using a space velocity (GHSV) of 25000 h-1. The characteristics of catalysts and the state of copper ions in CuHY and CuHMFI containing additions of V or



Cs, were evaluated by XRD and H2-TPR. The light-off temperatures (T50% toluene conversion into CO2) determined for CuHMFI are lower than for CuHY, which means that CuHMFI based catalyst are more active for complete oxidation of toluene than CuHY with similar

copper contents. This difference of activity is associated to an increase of copper reducibility in MFI zeolite. For both types of zeolites, the activity increases with the copper content, but for MFI with 2 and 5 wt.% the light-off temperatures are very similar, therefore it is not profitable to use catalysts with higher metal contents, our studies have proceeded based on CuMFI with about 2 wt.%. For this catalyst, the addition of V and Cs leads to a decrease in the light-off temperature of 35ºC and 50ºC respectively. But while in the presence of V, the catalyst evidences some selectivity to CO, in presence of Cs the selectivity into CO2 is 100 %. The Cs presence increases the reducibility of Cu species and also affects the Cu^{2+} ions position in the zeolite.

PROCESSING OF CORDIERITE FOAMS BY DIRECT FOAMING

Silva, Elisabete R.[1]; Correia, Nuno[2]; Silva, João M.[2]; Oliveira, Fernando C.[3]; Ribeiro, F. Ramôa[1]; Bordado, João C.[1]; Ribeiro, M. Filipa[1]

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Open-cell ceramic foams have properties that make them attractive as catalyst supports. The "replication" process is the most widely and versatile method used for producing cellular ceramic materials. One of the drawbacks of this process is that the ceramic ligaments (struts) contain a hollow cavity possessing sharp edges due to the burnout of the polymeric template. The presence of such voids in the struts decreases the cohesion of the material in comparison to foams possessing dense struts manufactured by conventional direct foaming techniques. The aim of this work was therefore to develop cordierite-based foams by a direct foaming method and to compare the resulting properties with those obtained for foams previously developed by the replication process. The ultimate goal is to fabricate supports for depositing metal zeolites suitable for catalytic combustion of VOCs.In this work reticulated cordierite foams have been prepared by mixing of ceramic particles within a polyol followed by reaction with a MDI type isocyanate to form a polyurethane foam. Some of the experimental parameters, which were optimized, include the type and amount of surfactant, catalyst, polyol as well as the content of solids, plasticizer and blowing agent that need to be added. After curing, the polymer was burnt out under air, and the resulting ceramic foam was then sintered.Up to now, foams possessing porosities higher than 90% were obtained. Efforts are being made in order to increase density by adding coupling agents to promote a better dispersion of the inorganic filler within the polymer mix. The presence of surfactant has been found to play an important role in stabilizing the liquid-gas interface of bubbles during the expansion step, thus affecting significantly the cell characteristics of the resulting cordierite foams. Alternative ways for controlling foam density are discussed.

Publicado em:
Proceedings of E-MRS 2006 Fall Meeting, Warsaw, Poland, September 2006

"ULTRAFILTRATION AND PHYSICAL-CHEMICAL/ULTRAFILTRATION TREATMENTS FOR THE CORK PROCESSING WASTEWATERS"

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Membrane fouling is the major problem in the treatment by ultrafiltration (UF) of the cork processing wastewaters. This problem leads to drastic reduction on the permeate fluxes and has been associated to the wastewaters phenolic/tannic colloidal matter (Minhalma et al. 2000). In order to minimize UF fouling several membrane pre-treatments were investigated. The physical-chemical pre-treatments tested were: flocculation/flotation; Ozonization.

A flocculation study was carried out with chitosan. A Dissolved-Air-Flotation (DAF) study was performed with the wastewater clarified by flocculation. The parameters varied were the operating pressure and the recycle-ratio. It was observed that for higher pressures and at a recycle-ratio of 0.19 the polyphenols removal was maximal.

The ozonation pre-treatment was conducted with the objective of oxidizing selectively phenolic compounds and subsequently obtain higher UF permeate fluxes.

The flocculation/flotation pre-treatment led to the enhancement of the UF permeate fluxes. For the membrane with higher MWCO, CA4, the permeate flux enhancement reached the 130%.

The ozone pre-treatment led to a reduction of 11% in the total organic carbon content and to a reduction of 51% in the total polyphenols content, these reductions led to the enhancement of the UF permeate fluxes in 40%.

The physical-chemical pre-treatments tested (flocculation/flotation and Ozonization) shown very positive results that allowed the ultrafiltration to present much higher fluxes and therefore became a very attractive operation for the treatment/valorization of the cork processing wastewaters.

"CONTROL OF GASEOUS EMISSIONS IN ARC WELDING"

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A health and safety environment is considered determinant for the use of arc welding. This paper describes a the effects of shielding gas composition on the amount of welding fume produced, its composition and particle size, during Gas Metal Arc Welding which is the most common and the one that produces the largest amount of fume, using a wide range of welding parameters. This topic is of great international concern, which is reflected by a recently approved project by the EC, entitled Econoweld. This project aims at enhancing productivity in combination with a reduction of sick leave among welders, by improving workshop ergonomics and by reducing the welding fume emission of the GMAW process. Contributions for a better understanding of fume formation and its effect on the atmosphere around the welders are of significant relevance for the case of these technologies and are presented in this paper.

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Proceedings da 6th European Conference on Welding, Cutting and Joining Technologies, Santiago de Compostela, Espanha, 28 a 30 Junho 2006

"EVALUATION OF GASEOUS EMISSIONS OF OIL AND GAS BOILERS FROM PORTUGUESE INDUSTRY"

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Publicado em:
Proceedings da INFUB7 – 7th European Conference on Industrial Furnaces and Boilers, Porto, 18 a 21 Abril 2006

This paper describes a study on the evaluation of the atmospheric emissions from oil and gas boilers installed in the Portuguese industry. Atmospheric emissions were measured in terms of total suspended particulate, sulphur dioxide, nitrogen oxides, carbon monoxide and volatile organic compounds, as well as characteristic gaseous flow parameters, such as temperature, pressure and velocity; and are critically compared with the allowable emission levels.
This obtained information is also evaluated considering the new revised Portuguese regulations on air emissions.

"OUTLINE OF A METHODOLOGY FOR CONSTRUCTION OF A HEALTHY BUILDING"

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This work describes the outline of a methodology, which has been applied with success in several situations, for construction of a healthy building in terms of Indoor Air Quality (IAQ). This methodology aims to decrease or even eliminate, where possible, the emissions resulting from building materials and includes the following steps: the evaluation of available information and specifications on building materials and related products; discussions with manufacturers, analysis of samples, in situ inspections and final IAQ investigations. An outline of this methodology is presented in figure 1.

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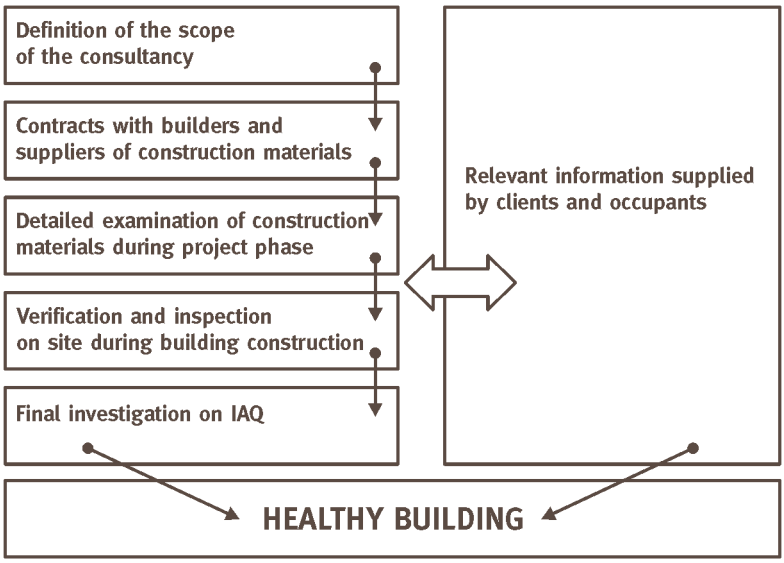

Figure 1. Description of the methodology

"SYNTHESIS OF NEW ABSORBENTS FOR EFFECTIVE FOREST FIGHTING"

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Publicado em:
Proceedings do XX Encontro Nacional da Sociedade Portuguesa de Química, Almada, 14 a 16 de Dezembro, 2006

Currently, the most frequently used fire-fighting medium is still water, and its extinguishing properties are based primarily on its cooling effect, cooling down the combustible material below ignition point. Thus, water takes up the heat and removes it to a certain extent with the steam. Nevertheless, what happens is that water does not stay in the area where it is dropped, as around 95% run-off on surface and is absorbed by soil. Therefore, a higher amount of water is required due to an inefficient use. As it is well known, water is a very critical resource in wild land, which makes that, when it is used for fire extinction, an efficient use is critical. Also, run-off water may contain toxic and harmful chemicals from the burned material itself. The synthesis of new superabsorbent polymers has been dealt with, and their synthesis has been optimised bearing in mind this particular application, that is for the production of water insoluble polymers having high water absorption capacity. For this purpose, polymers should have functional groups with high compatibility with water, such as OH, COOH and SO_3H. Therefore, the developed polymer is called AMPS: 2-acrylamide-2-methyl-propane-sulphonic, and its general formula for its monomer is: $CH_2{=}CHCONHC(CH_3)_2CH_2SO_3H$. The homopolymer has been synthetised from the hydrophilic monomer AMPS, and forms copolymers with acrylamide (AA) and AA/AMPS with bis-acrylamide (BA) as a crosslinking agent. The polymerisation followed a free radical technique in the presence of potassium persulphate. The most interesting property of a superabsorbent polymer, from the application point of view, is its absorption capacity. A polymeric material having superabsorbent characteristics, immersed in a water media interacts with the solvent molecules, trapping them and leading to the polymer swelling. The interaction between polymer and solvent molecules is due to a good thermodynamic compatibility, which allows the expansion of the polymer texture forming a state similar to a solution. The influence of several structural parameters on the swelling properties of these superabsorbents has been studied. Experimentally, the effects of polymer composition such as the fraction of used monomer and the content of crosslinking agent on swelling were also deter-

mined, in order to optimise the polymer considering this application. It can be noticed that there is a high dependence of the swelling capability with the amount of AMPS: the swelling ratio increases as the amount of AMPS increases until a maximum of 1240, obtained for 30% of AMPS and then decreases slightly. This behaviour is observed as, by increasing the concentration of ionizing groups in the polymer network, the osmotic pressure of the polymer increases and it expands. However, for more than 30% of AMPS, the swelling capacity decreases which is due to the difficulty of ionizing the polymer. Regarding the amount of crosslinking agent BA, the effect on polymer swelling was also investigated. The obtained results indicate the formation of gels from water soluble to insoluble. For low crosslinking agent added the polymer is soluble, but, for increasing quantities, the solubility reduces and the copolymer is absorbent. For high concentrations of crosslinking agent, the polymerization conditions are affected and other types of polymers are formed which explains the observed solubility. This data allowed to determine the optimum conditions for the synthesis of this polymer, for water absorption, as 30% of AMPS and 70% of acrylamide, using 0,5% of bis-acrylamide as cross linking agent.

Superabsorbent swelled polymer, which have more than 1 liter of water per gram of polymer is somehow like “solidified water”. Up to 30 to 40% of swelled gel particles do not affect significantly the apparent viscosity and can be handled by conventional fire extinguishing pump systems. The main advantage is that a large part of these gel particles will remain on the top of the leaves and branches of trees and are much more effective in cooling than the thin film of flowing water that, in most cases do not even wets the hydrophobic surface of the leaves.

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"SYNTHESIS AND CHARACTERISATION OF HYDROXYAPATITE"

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Hydroxyapatite (HAP), is represented by the formula $Ca_{10}(PO_4)_6(OH)_2$, and is one of the inorganic components of the hard tissues of living bodies such as bones and teeth. HAP is a calcium phosphate based bio-ceramic, which has been used for several years in medicine and dentistry because of its excellent biocompatibility with human tissues. The success of its application in these fields depends upon factors such as the composition, crystallinity, size and morphology of HAP particles. This paper describes the work performed regarding the synthesis of this compound by a wet method comprising the direct precipitation of orthophosphoric acid solution to a calcium hydroxide solution, the process being described by the following reaction: 10 $Ca(OH)_2$ + 6 $H_3(PO_4)$ ‹=› $Ca_{10}(PO_4)_6(OH)_2$ + 18 H_2O. Synthesis was performed in a laboratory reactor, 700 mL in capacity, instrumented and controlled using a computer interface, so that the influence on process variables such as reaction temperature, pH, medium inertization by N_2, velocity of stirring and the flow rate input of $H_3(PO_4)$, could be assessed. The influence of these parameters was, therefore, evaluated in terms of the required composition and morphology of HAP formed particles, analysing them by FTIR, XRD, SEM and EPMA for determination of the Ca/P ratio. From the obtained results, it can be concluded that HAP particles having suitable properties for use in medicine, could effectively be prepared by this technique, provided that a good control of the involved process variables is maintained.
This preliminary work is part of a broader study aiming to the scale-up of the reactor.

SYNTHESIS AND Rh(I)-CATALYZED POLYMERIZATION OF 1,3-DIPHENYLYNE-CALIX[4]ARENE COMPOUNDS: NOVEL CONJUGATED, CALIXARENE-BASED POLYMERS

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The synthesis of two 1,3-bis(4-ethynylbenzyloxy)calix[4]arenes, 5,11, 17,23-tetrakis(1,1-dimethylethyl)-25,27-bis(4-ethynylbenzyloxy)-26,28-dihydroxy-calix[4]arene **(1)** and 25,27-bis(4-ethynylbenzyloxy)-26,28-dihydroxycalix[4]arene **(2)**, was accomplished through Sonogashira coupling of appropriate calixarene derivatives. Methods for the polymerization of these bifunctional building blocks with Rh(I) as a catalyst, leading ultimately to conjugated polymers having calix[4]arene units incorporated into the main chain, were explored. Calixarenes **1** and **2** were efficiently polymerized with rhodium-based initiators and afforded the conjugated polymers poly{5,11,17,23-tetrakis(1,1-dimethylethyl)-25,27-bis(4-ethynylben-zyloxy)-26,28-dihydroxycalix[4]arene} (**poly 1**) and poly{25,27-bis(4-ethynylbenzyloxy)-26,28-dihydroxycalix[4]arene}. Depending on the conditions, high conversions and good yields were obtained. The effects of adding cocatalysts ($NHEt_2$ and/or PPh_3) were studied in connection with the number-average molecular weight and the molecular weight distribution of the resultant polymer (**poly 1**) and tentatively correlated with the formation of low-molecular-weight materials. A catalytic system containing triphenylphosphine as the sole additive ($[Rh(nbd)Cl]_2$; $[Rh]/[PPh_3]=0.5$) proved to be the best for the polymerization of p-tert-butylcalixarene compound 1. Linear polymers having high number-average molecular weights (up to $1.1 ¥ 10^5$ g mol^{-1}) with low polydispersities were produced under these conditions. For debutylated homologue **2**, its polymerization was best carried out in the absence of any added cocatalyst. A cyclopolymerization route, comprising the intramolecular ring closing of the calix[4]arene pendant ethynyl groups followed by an intermolecular propagation step, is advanced to explain the results.

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Journal of Polymer Science Part A-Polymer Chemistry, 2006, 44, 7054-7070

COMPARATIVE STUDY OF THE COPOLYMERIZATION KINETICS OF MONO AND DIVINYLBENZYL p-TERT-BUTYLCALIX[4]ARENE DERIVATIVES AND STYRENE

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Supramolecular Chemistry, 2006, 18, 191-198

A study of the copolymerization kinetics of 25,27-bis-(4-vinyl-benzyloxy)-26,28-dihydroxy-*p-tert*-butylcalix[4]arene (**1**) and 25,26,27-tripropoxy-28-(4-vinyl-benzyloxy)-*p-tert*-butylcalix[4]arene (**2**) with styrene (**St**) was undertaken. The radical copolymerizations were carried out in THF in the presence of benzoyl peroxide at 75ºC for a certain period. Six molar feed ratios, ranging from 1:1 to 1:20 (**1** or **2** to **St**), were used to calculate the reactivity parameters. The copolymer composition was determined by FT-IR spectroscopy using a Beer's law plot obtained from the corresponding homopolymers. The reactivity ratio calculations were performed with the linearization methods of Fineman-Ross (F-R) and Kelen-Tüdös (K-T), assuming the validity of the so-called terminal model. In the copolymerization of the monoene **2**, similar reactivity ratios were found for the comonomers (*ca.* 1.2; K-T). On the other hand, the reactivity ratios calculated for the copolymerization of **1** with **St** yielded r_{St} = 0.67 and r_{calix} = 3.0 (K-T method). The higher reactivity of monomer **1** as compared to styrene is discussed in connection with our previously postulated cyclocopolymerization route.

RADICAL CYCLOPOLYMERIZATION OF A DIVINYLBENZYL-p-TERT-BUTYL-CALIX[4]ARENE DERIVATIVE

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The synthesis and characterization of a new homopolymer (**poly 1**), obtained in the course of the radical polymerization of 25,27-bis-(4-vinyl-benzyloxy)-26,28-dihydroxy-*p-tert*-butylcalix[4]arene (1), is described. Homopolymerization of **1** in THF, using BPO or thermal initiation, afforded soluble polymers in good isolated yields (60-90%). Gel permeation chromatography (GPC) profiles showed unimodal distributions for all the analyzed polymers, which is indicative that chain branching reactions did not occur to a major extent. Molecular weights (M_n) ranging from 30000-60000 $gmol^{-1}$ were reached within a 8h period, when the reactions were conducted at 0.06-0.5 mol% of BPO or thermally initiated, showing relatively narrow polydispersity indexes (1.5-2.0). The structure of the polymers was deduced upon analysis of their ^1H NMR and FT-IR spectra, which, in conjunction with GPC and solubility data led to their formulation as cyclopolymers.

Publicado em:
Reactive and Functional Polymers, 2006, 66, 465-470

ISOLATION AND COMPARATIVE CHARACTERIZATION OF A BJÖRKMAN LIGNIN FROM THE SAPONIFIED CORK OF DOUGLAS FIR BARK

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Cork from Douglas-fir bark (*Pseudotsuga menziesii*) was separated, extracted and submitted to suberin depolymerization by transesterification with sodium methoxide in methanol. As a result a saponified cork fraction ($cork_{sap}$) with a yield of 19% was obtained. From $cork_{sap}$ a milled cork lignin (MCL_{sap}) was isolated using the Björkman procedure with a yield of 0.75% (based on $cork_{sap}$, corresponding to 0.14% based on original cork). The isolated Douglas-fir MCL_{sap} was characterized by elemental analysis and OMe determination, FT-IR spectroscopy and analytical pyrolysis (Py-GC/FID). Data are presented in comparison with those of MCL_{sap} isolated from cork-oak (*Quercus suber*) and milled wood lignins (MWL) of spruce. All data revealed that the Douglas-fir cork lignin has a guaiacyl-type structure (G-lignin). Results of Py-GC/FID demonstrate that this polymer consists of approx. 97% guaiacyl, 2% p-hydroxyphenyl and 1% syringyl units.

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

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

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Wood Science and Technology, 2006 (Online first. DOI: 10.1007/s00226-006-0099-0)

KINETIC PROPERTIES OF WILD-TYPE AND ALTERED RECOMBINANT AMIDASES BY THE USE OF ION--SELECTIVE ELECTRODE ASSAY METHOD

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A novel assay method was investigated for wild-type and recombinant mutant amidases (EC 3.5.1.4) from *Pseudomonas aeruginosa* by ammonium ion-selective electrode (ISE). The initial velocity is proportional to the enzyme concentration by using the wild-type enzyme. The specific activities of the purified amidase were found to be 88.2 and 104.2 U mg protein^{-1} for the linked assay and ISE methods, respectively. The kinetic constants—V_{max}, K_m, and K_{cat}—determined by Michaelis–Menten plot were 101.13 U mg protein^{-1}, 1.12 x 10^{-2} M, and 64.04 s^{-1}, respectively, for acrylamide as the substrate. On the other hand, the lower limit of detection and range of linearity of enzyme concentration were found to be 10.8 and 10.8 to 500 ng, respectively, for the linked assay method and 15.0 and 15.0 to 15,000 ng, respectively, for the ISE method. Hydroxylamine was found to act as an uncompetitive activator of hydrolysis reaction catalyzed by amidase given that there is an increase in V_{max} and K_m when acetamide was used as the substrate. However, the effect of hydroxylamine on the hydrolysis reaction was dependent on the type of amidase and substrate involved in the reaction mixture. The degrees of activation (ε_a) of the wild-type and mutant (T103I and C91A) enzymes were found to be 2.54, 12.63, and 4.33, respectively, for acetamide as the substrate. However, hydroxylamine did not activate the reaction catalyzed by wild-type and altered (C91A and W138G) amidases by using acrylamide and acetamide, respectively, as the substrate. The activating effect of hydroxylamine on the hydrolysis of acetamide, acrylamide, and *p*-nitrophenylacetamide can be explained by the fact that additional formation of ammonium ions occurred due to the transferase activity of amidases. However, the activating effect of hydroxylamine on the hydrolysis of *p*-nitroacetanilide may be due to a change in conformation of enzyme molecule. Therefore, the use of ISE permitted the study of the kinetic properties of wild-type and mutant amidases because it was possible to measure initial velocity of the enzyme-catalyzed reaction in real time.

SCREENING OF SUITABLE IMMOBILIZED METAL CHELATES FOR ADSORPTION OF MONOCLONAL ANTIBODIES AGAINST MUTANT AMIDASE FROM PSEUDOMONAS AERUGINOSA

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ABSTRACT

The chromatographic behaviour of monoclonal antibodies (MAbs) of IgM class against mutant (T103I) amidase from *Pseudomonas aeruginosa* was investigated. The effect of ligand concentration, the length of spacer arm and the nature of metal ion were investigated on immobilized metal ion affinity chromatography (IMAC). MAbs against mutant amidase adsorbed to Cu (II), Ni (II), Zn (II), Co (II) and Ca (II)-IDA agarose columns. The adsorption of MAbs onto immobilized metal chelates was pH dependent because an increase in the binding of MAbs was observed as the pH was raised from 6.0 to 8.0. The adsorption of MAbs to metal chelates was due to coordination of histidine residues which are available in the 3rd constant domain of heavy chain (CH3) of immunoglobulins since the presence of imidazole in the equilibration buffer abolished the adsorption of MAbs to the column packed with commercial IDA-Zn(II) agarose at pH 8.0. The combination of tailor-made stationary phases for IMAC and a correct choice of the adsorption conditions permitted to design a one-step purification procedure for MAbs of IgM class. Culture supernatants containing MAbs of IgM class against mutant amidase (T103I) were chromatographed by IMAC Co (II) column at pH 8.0. The results strongly suggest that one-step purification of MAbs of IgM class by IMAC is a cost-effective and process-compatible alternative to the other purification procedures.

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IMMOBILIZED METAL AFFINITY CHROMATOGRAPHY OF MONOCLONAL IMMUNOGLOBULIN M AGAINST MUTANT AMIDASE FROM PSEUDOMONAS AERUGINOSA

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The chromatographic behavior of monoclonal antibodies (MAbs) of immunoglobulin (Ig) M class against mutant (T103I) amidase from *Pseudomonas aeruginosa* was investigated on immobilized metal chelates. The effect of ligand concentration, the length of spacer arm, and the nature of metal ion were investigated in immobilized metal affinity chromatography (IMAC). The MAbs against mutant amidase adsorbed to Cu(II), Ni(II), Zn(II), Co(II), and Ca(II)-iminodiacetic acid (IDA) agarose columns. The increase in ligand concentration (epichlorohydrin: 30–60 and 1,4-butanediol-diglycidyl ether: 16–36) resulted in higher adsorption to IgM into immobilized metal chelates. The length of spacer arm was found to affect protein adsorption, as longer spacer arm (i.e., 1,4-butanediol-diglycidyl ether) increased protein adsorption of immobilized metal chelates. The adsorption of IgM onto immobilized metal chelates was pH dependent because an increase in the binding of IgM was observed as the pH varied from 6.0 to 8.0. The adsorption of IgM to immobilized metal chelates was the result of coordination of histidine residues to metal chelates that are available in the third constant domain of heavy chain (CH3) of immunoglobulins, as the presence of imidazole (5 mM) in the equilibration buffer abolished the adsorption of IgM to the column. The combination of tailor-made stationary phases for IMAC and a correct design of the adsorption parameters permitted to devise a one-step purification procedure for IgM. Culture supernatants containing IgM against mutant amidase (T103I) were purified either by IMAC on EPI-60–IDA-Co (II) column or by gel filtration chromatography on Sephacryl S-300HR. The specific content of IgM and final recovery of antibody activity exhibited similar values for both purification schemes. The purified preparations of IgM obtained by both schemes were apparently homogeneous on native polyacrylamide gel electrophoresis with a M_r of 851,000 Da. The results presented in this work strongly suggest that one-step purification of IgM by IMAC is a cost-effective and processcompatible alternative to other types of chromatography.

HYDROISOMERIZATION OF N-HEXANE OVER PT–NI/HBEA USING CATALYSTS PREPARED BY DIFFERENT METHODS

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Bimetallic catalysts Pt-Ni/HBEA prepared by different methods, were studied in the reaction of n-hexane hydroisomerization and compared with Pt and Ni/HBEA. The results showed that the highest conversion and selectivity were obtained for the bimetallic catalysts, prepared by ion exchange with simultaneous addition of Pt and Ni, which reveals a synergistic effect between the two metals.

Publicado em:
Catalysis Letters, 2006, 109, 83-87

SUPPORTED PYRAZOL RHENIUM COMPLEXES AS CATALYSTS FOR CYCLOHEXANE OXIDATION BY MOLECULAR OXYGEN

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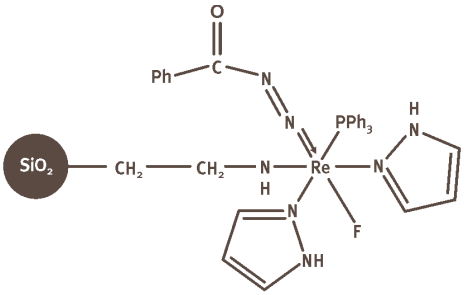
Publicado em:
Livro de Abstracts da VII[th] Netherlands' Catalysis and Chemistry Conference, Noordwijkerhout, Holanda, Março de 2006

Heterogeneous catalysis provides eco-friendly methods [1] for the synthesis of fine chemicals and pharmaceuticals [2], since the use of he-terogeneous catalysts, in comparison with homogeneous ones, allows easier separation, recovery and recycling and can also lead to a good selectivity. The oxidation of cyclohexane [3] forms products, viz. cyclohexanone and cyclohexanol, that are key intermediates in the manufacture of nylon-6,6. In the current context, we have anchored some pyrazole rhenium(III) and (V) complexes to 3-aminopropyl functionalized silica gel, and tested their use for the catalytic oxidation of cyclohexane. The expected structure of the final supported $[ReClF\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ catalyst is given below (the other Re complexes should be similarly anchored).



These supported rhenium complexes serve as effective heterogeneous catalysts for cyclohexane oxidation in the presence of dioxygen without any additive. The supported $[ReClF\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ complex gives the best yield (11%) and good selectivity for cyclohexanone and cyclohexanol, which is further promoted by the presence of some he-teroaromatic acids such as the 2-pyrazinecarboxylic acid. The reaction occurs under relatively mild conditions (150 oC, 13.6 atm O_2 for 8 h). TGA shows that the catalysts are stable at the reaction temperature and the morphology of the catalyst was analyzed by SEM. Evidence is presented in favour of the involvement of a free-radical mechanism. A comparison with the activity of some homogeneous Re catalysts we have recently reported [4] will also be provided.

SYNTHESIS AND ELECTROCHEMICAL BEHAVIOUR OF SCORPIONATE IRON COMPLEXES

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The coordination chemistry of tridentate nitrogen donor ligands has been developed in the last years namely due to the applications of their complexes in industrial and biological processes. However, in contrast to the widely studied anionic hydrotris(1-pyrazolyl)borate ($HBpz_3^-$, Tp; pz = pyrazolyl), the coordination chemistry of the isoelectronic N_3 tripodal neutral hydrotris(1-pyrazolyl)methane ($HCpz_3$, Tpm) or of the tris(1-pyrazolyl)methanesulfonate ($SO_3Cpz_3^-$, Tpms) (with an increased solubility in polar solvents and higher resistance to hydrolysis, in comparison with Tp) has been much less investigated and still constitutes an underdeveloped field of research.

We now report the reactions of $HBpz_3$, $HCpz_3$ and $Li[SO_3Cpz_3]$ with iron(II) centres, leading to the complex double salt $[Fe(HBpz_3)_2][FeCl_4]$ and to the half-sandwich hydrotris(pyrazolyl)methane $[FeCl_2(HCpz_3)]$ and tris(1-pyrazolyl)methanesulfonate $Li[FeCl_2(SO_3Cpz_3)]$ compounds. The new complexes have been characterized by IR and multinuclear NMR spectroscopies, FAB-MS spectrometry and elemental analysis.

The electrochemical behaviour of the above complexes, as studied by cyclic voltammetry (CV) at a Pt-disc electrode and by controlled potential electrolysis (CPE) at a Pt-gauze electrode, is now reported. The obtained electrochemical results are discussed in terms of electron richness of the Fe centres and the electronic properties of the ligands.

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TRIS(1-PYRAZOLYL)METHANE AND DERIVED VANADIUM COMPLEXES MIMICKING THE CATALYTIC ACTIVITY OF AMAVADINE

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Livro de Abstracts do EUROBIC 8 - 8th European Biological Chemistry Conference and EUROBIC Young Researchers Forum, Aveiro, Portugal, Julho de 2006.

Amavadine, a natural vanadium complex present in some *Amanita muscaria* fungi, whose biological function is still unknown, can exhibit haloperoxidase- and peroxidase-type activities, and act as catalyst for the oxidation of some biological thiols, for the peroxidative halogenation, hydroxylation, and oxo-functionalization of alkanes and aromatic compounds.[1] These findings gave rise to new experiments with its synthetic analogues and other V complexes with N,O-ligands, as catalysts for the functionalisation of alkanes (including CH_4) and aromatics in mild conditions.

In pursuit of the aim to understand the biological role of Amavadine and its application on reactions with potential industrial interest, here we report the extension of the above studies to the catalytical conversion of methane to acetic acid, in the presence of $V^{(III-V)}$ complexes with the N_3 tripodal tris(1-pyrazolyl)methane ($HCpz_3$) or tris(1-pyrazolyl)methanesulfonate ($SO_3Cpz_3^-$) ligand, using $K_2S_2O_8$ as an oxidant and (CF_3COOH) TFA as a solvent. Turnover numbers and yields are reported, as well as the effects of pressure of methane, amount of catalyst, type of oxidant and presence of a radical trap.

SOME COPPER AND VANADIUM TRIS(PYRAZOLYL)METHANE COMPLEXES AS CATALYSTS FOR THE PEROXIDATIVE OXIDATION OF CYCLOALKANES

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Following our studies on the peroxidative oxidation of cyclohexane catalysed by V and polynuclear Cu complexes with N,O ligands, we now report the synthesis of new complexes with these metals but with tripodal ligands hydrotris(pyrazolyl)methane and derived sulfonate and show that they act as catalysts in the peroxidative oxidation of alkanes to the corresponding alcohols and ketones, under mild conditions in aqueous/acetonitrile medium. The complexes have been characterized by IR and multinuclear NMR or EPR spectroscopies, FAB-MS and elemental analysis.

The turnover numbers and yields are indicated and the effects of various factors *e.g.* relative amounts of catalyst, substrate and oxidant, type of oxidant, solvent, presence of radical traps, reaction time and temperature are reported.

Publicado em:
Livro de Abstracts do 1st European Chemistry Congress, Budapeste, Hungria, Agosto de 2006

SCORPIONATE IRON COMPLEXES AS CATALYSTS FOR THE PEROXIDATIVE OXIDATION OF CYCLOHEXANE IN AQUEOUS MEDIUM

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Livro de Abstracts da 1st International IUPAC Conference on Green-Sustainable Chemistry, Dresden, Alemanha, Setembro de 2006

The oxidation of cyclohexane is a rather important process due to the large demand for its oxidized products, cyclohexanol and cyclohexanone, which are commodity chemicals used as intermediates *e.g.*, in the manufacture of adipic acid, nylon-6,6', polyamide-6, urethane foams, and lubricant additives.

In normal industrial catalytic systems, which employ cobalt salts, molecular oxygen and temperatures above 150 ºC, low conversion is obtained and many efforts have been made to develop new catalysts to oxidize cyclohexane under mild conditions with high selectivity and yield, using different oxidizing agents.

Herein we report the synthesis of new iron complexes with the N_3 tripodal ligands hydrotris(1-pyrazolyl)borate ($HBpz_3^-$, pz = pyrazolyl, Tp), hydrotris(1-pyrazolyl)methane ($HCpz_3$, Tpm) and tris(1-pyrazolyl) methanesulfonate ($SO_3Cpz_3^-$,Tpms), and their catalytic activity in the peroxidative oxidation of cyclohexane to the corresponding alchool and ketone, under mild conditions (*e.g.*, room temperature, normal pressure), in aqueous medium with an environmentally friendly oxidant (H_2O_2 that produces only water as by-product).

The new complexes have been characterized by IR and multinuclear NMR spectroscopies, X-ray diffraction, FAB-MS spectrometry and elemental analysis. Turnover numbers and yields are indicated as well as the effects on the catalytic activity of various factors such as the relative amounts of catalyst, substrate, oxidant, type of oxidant, solvent, presence of radical traps, reaction time and temperature.

ELECTROCHEMICAL PROPERTIES OF SCORPIONATE VANADIUM COMPLEXES, CATALYSTS FOR OXIDATION OF ALKANES

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In pursuit of our interest on transition-metal-catalysed functionalization of alkanes, in particular the selective oxidation of lower alkanes to high added value chemicals, we have found that hydrotris(1-pyrazolyl) methane ($HCpz_3$, Tpm) and tris(1-pyrazolyl)methanesulfonate ($SO_3Cpz_3^-$, Tpms) vanadium(IV and V) complexes such as $[VOCl(SO_3Cpz_3)]$, $[VCl_2(SO_3Cpz_3)]Cl$ and $[VO(SO_3Cpz_3)][BF_4]_2$ can act as catalysts in the peroxidative oxidation of cyclohexane to the corresponding alcohol and ketone, as well as in the oxidation of methane to acetic acid, under mild conditions.

We now report the electrochemical behaviour of the above complexes, as studied by cyclic voltammetry (CV) at a Pt-disc electrode and by controlled potential electrolysis (CPE) at a Pt-gauze electrode. The obtained electrochemical results are discussed in terms of electron richness of the vanadium centres and the electronic properties of the ligands.

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Livro de Abstracts das Jornadas de Electroquímica e Inovação 2006, Porto, Portugal, Outubro de 2006

IN THE ROUTE FOR A SUSTAINABLE CHEMICAL PROCESS: NEW VANADIUM CATALYSTS FOR THE CARBOXYLATION OF ETHANE

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Publicado em:
Livro de Abstracts do XX Encontro Nacional da Sociedade Portuguesa de Química, Caparica, Portugal, Dezembro de 2006

There are many challenges facing synthetic chemists in the drive towards the development of new processes for a more sustainable future. Amongst current approaches, homogeneous catalysis is of prime importance and it has been our interest to find new transition-metal catalysts for the functionalization of lower alkanes under mild conditions in view of the potential significance of such organic compounds as raw materials for synthesis and of the commercial value of the products.

Here in we report the catalytic oxidation of ethane to acetic and/or propionic acid, in a single-pot process and under mild conditions, by vanadium(III-V) complexes with the N_3 tripodal tris(1-pyrazolyl) methane ($HCpz_3$) or tris(1-pyrazolyl)methanesulfonate ($SO_3Cpz_3^-$) ligand, in the presence of the peroxodisulfate salt $K_2S_2O_8$ as the oxidizing agent and in trifluoroacetic acid as the solvent:

$$C_2H_6 \xrightarrow[K_2S_2O_8,\ CF_3COOH]{\text{V catalyst}} CH_3COOH + C_2H_5COOH$$

Reaction conditions, turnover numbers and yields are reported.

ORGANOMETALLIC NONLINEAR OPTICAL COMPLEXES: A TUNABLE WAVELENGTH HYPER-RAYLEIGH SCATTERING STUDY

Wenseleers, W.[1]; Campo, J.[1]; Goovaerts, E.[1]; Robalo, M. Paula[2,3]; Teixeira, A.P.S.[2,4]; Garcia, M.H.[2,5]; Dias, A.R.[2]

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Organic and organometallic molecules have been examined intensively in the search for new materials with improved second-order nonlinear optical (NLO) properties, for applications such as parametric frequency conversion and electro-optic modulators. Studies of systematically varied series of nitrile complexes, correlating molecular structure, hyperpolarizability β, and spectroscopic properties, have led to the development of complexes with very large molecular hyperpolarizabilities. In particular, we recently found that pseudo-octahedral hydrido(nitrile)iron(II) complexes possess even higher hyperpolarizabilities than analogous cyclopentadienyl complexes. However, as absorption wavelengths of the optimized NLO complexes shift further to the red, it becomes increasingly important to take into account the resonance effects on β. The two-level β dispersion model of Oudar and Chemla (TLM),[3] which is widely used in literature to extrapolate resonant β values to the static limit, ignores line broadening and is therefore expected to become invalid close to resonance. To examine the dispersion of b experimentally in both the resonance and the non-resonance region we perform wavelength-dependent hyper-Rayleigh scattering (HRS) measurements using the tunable output from a picosecond optical parametric amplifier (OPA) and registering the HRS light with an intensified CCD. This detector yields a nanosecond gated, parallel registration of a ~23 nm spectral region around the second harmonic wavelength enabling correction for multi-photon fluorescence, and its single-photon sensitivity allows for an accurate internal calibration against the pure solvent even at long wavelengths. The molecular β for two pseudo-octahedral hydrido(nitrile)iron(II) complexes, determined in the 1072-1580 nm range (Fig. 1), reveals a pronounced two-photon resonance with the charge-transfer (CT) state in both cases. The TLM curves based on the most resonant (1072 nm) and the least resonant β value (1540 nm, shown for **1** only) are also plotted in Figure 1. While the TLM appears to give a reasonable description of the β dispersion of compound **2**, even at 1072 nm, the undamped TLM clearly fails for the more resonant compound **1**, and would be totally inadequate to derive the static β_0 from β at 1072 nm.

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Livro de Abstracts da International Conference on Organic Photonics and Electronics 2006 (ICOPE2006) & 9th International Conference on Organic Nonlinear Optics (ICONO'9), Brugges, Bélgica, Setembro de 2006

To give a satisfactory description of the dispersion, (in) homogeneous line broadening needs to be incorporated somehow in the two-level model. In addition, the data for compound **1** suggests that multiple excited states and/or vibrational structure may need to be taken into account as well.

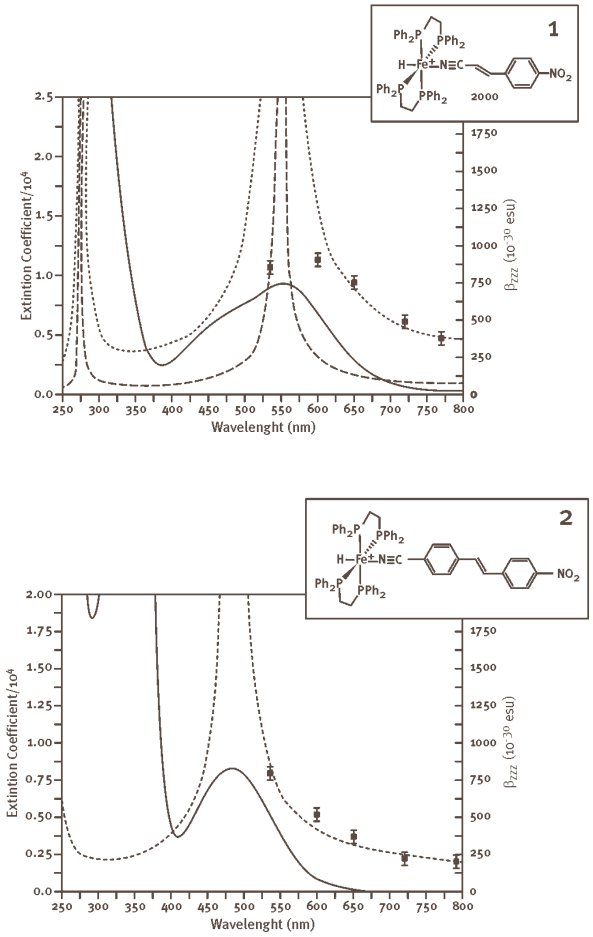

Figure 1: Experimental wavelength-dependent hyper-Rayleigh scattering (HRS) data (squares; shown at the second harmonic wavelength) for two pseudo-octahedral hydrido(nitrile)iron|(II) complexes (see insets) together with the absorption spectrum (solid line). Oudar-Chemla two-level model curves based on the most (dashed) and least resonant β values (dotted) are also shown (coincidentally overlapping for 2).

NEW IRON(II) AND RUTHENIUM(II) COMPLEXES WITH HELICALLY SHAPED SYSTEMS: SYNTHESIS AND CHARACTERIZATION

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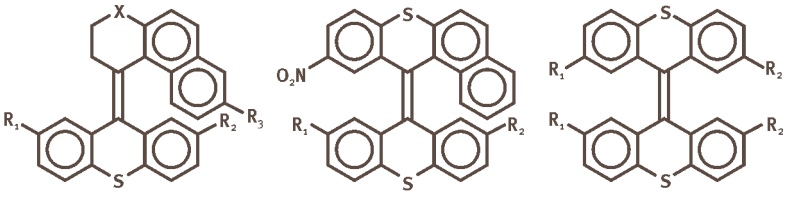
Publicado em:
Livro de Abstracts da XXII International Conference on Organometallic Chemistry, Zaragoza, Espanha, Julho de 2006

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

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

We report herein the synthesis and characterisation of organic overcrowded alkenes based in two building blocks, the thioxanthene and phenanthrene units and the coordination of these ligands to iron(II) and ruthenium(II) fragments, such as $[CpM(dppe)]^+$ (M = Fe(II), Ru(II)).



X = S, CH_2; R_1 = NC[M], CC[M]; [M] = $[Fe(\eta^5\text{-}C_5H_5)(dppe)]$, $[Ru(\eta^5\text{-}C_5H_5)(dppe)]$, $[Fe(dppe)_2(H)]$; R_2=NO_2; R_3= H, CH_3

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

SYNTHESIS OF NEW DITHIENYLETHENE IRON(II) AND RUTHENIUM(II) COMPLEXES: POTENTIAL PHOTOCHROMIC SWITCHES?

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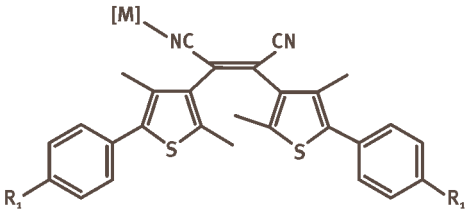
Publicado em:
Livro de Abstracts da XXII International Conference on Organometallic Chemistry, Zaragoza, Espanha, Julho de 2006

Photochromic molecules have attracted much attention due to their potential for applications to optical devices such as optical memories and switches. However, photochromic systems involving transition metal complexes has been very little explored, although the role of the transition metal centres has found to be relevant in the intramolecular photochromic process.

Among many known photochromic systems, diarylethenes containing five-membered heterocyclic rings received the most attention, since they are particularly well suited as switching units. Herein we report the synthesis and functionalisation of dithienylethene derivatives and their coordination to iron(II) and ruthenium(II) fragments, [M(η^5-C_5H_5)(dppe)] (M=Fe(II), Ru(II)) and [Fe(η^5-C_5H_5)$(CO)_2$] through nitrile group. The new complexes were characterised by the usual spectroscopic IR and NMR techniques and structural data discussed. Studies by UV/Vis spectroscopy were performed in order to characterise the photochromic behaviour of the compounds.



R1 = H, CN; [M] = [Fe(η^5-C_5H_5)(dppe)], [Ru(η^5-C_5H_5)(dppe)], [Fe(η^5-C_5H_5)$(CO)_2$]

STRUCTURAL CHARACTERIZATION OF THE TERTIARY MIXTURE METHANOL-ACETONITRILE-1-PROPANOL

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The study of solute-solvent-solvent interactions in mixed solvents has become increasingly important in the last few years due to the innumerous applications of this type of media in different processes. Although properties of binary mixtures have been extensively studied, very little work has been collected for ternary systems. However, these systems have a considerable interest in fields such as analytical chemistry, industrial processes and in the simulation design of biological environments.The present study aims at the structural characterizarion of the ternary mixture methanol/acetonitrile/1-propanol (MeOH/AcCN/1-PrOH), as a starting point to further reactivity and mechanistic studies. For this purpose we have determined the Dimroth and Reichardt parameter, *ETN*, and the refractive index, n_D, for 13 different compositions of the ternary system and for 10 different compositions of each of the 3 binary mixtures, at 25.0 and 50.0 ºC. The chemicals employed were supplied by Sigma-Aldrich (HPLC grade) and precautions were taken to avoid evaporation and contamination by humidity. We have applied the Bosch *et al*. preferential solvation model to the *ETN* data for the various binary mixtures. We have also calculated the excess quantities for the same mixtures. A variable-degree polynomial suggested by Redlich and Kister was used to correlate both excess properties for the binary mixture data. With the information thus collected, we have drawn some conclusions on the structure of the ternary system.

CORRELATION ANALYSIS APPLIED TO REACTIVITY STUDIES OF t-BuBr IN THE TERNARY MIXTURE METHANOL-1-PROPANOL-ACETONITRILE

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Publicado em:
Livro de Resumos do Workshop Mathematics In Chemistry, Lisboa, Portugal, 19 a 21 de Julho de 2006

Linear solvation energy relationships have been extensively used in the study of solvent effects, namely in correlations between kinetic data and solvents descriptors.
This approach is based in the premise that the logarithm of the rate constant, k, is proportional to the Gibbs energy of activation which can be divided into several contributions that either stabilize or destabilize the initial and/or the transition state. These contributions can be depicted through a set of carefully chosen and linearly related solvent descriptors:

$$\log k = a0 + a1\ (\text{descriptor 1}) + a2\ (\text{descriptor 2}) + \ldots$$

In the sequence of previous work, we now present rate constants values at 25.00 ºC, for the heterolysis of 2-bromo-2-methylpropane in a total of 79 mole fractions of the mixture methanol-1-propanol-acetonitrile.
The maximum wavelengths of 4-nitroanisole, 4-nitroaniline and 2,6-diphenyl-4-(2,4,6-triphenyl-1-pyridinio)-1-phenolate were also experimentally determined for the same mole fractions, thus allowing the determination of the solvent descriptors π^*, α and β.
The application of a correct methodology involving the assessment of any intercorrelations among the chosen descriptors, the use and proper choice of training and test sets, and the cautious selection of the best equation, based on accurate statistical criteria, allowed the identification and quantification of the main solute-solvent-solvent interactions influencing the reaction process under study.

CORROSION PERFORMANCE OF DOPED SILANE COATINGS AS PRE-TREATMENTS FOR MULTI SUBSTRATE APPLICATION

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Pre-treatments based on silane formulations lead to the formation of multifunctional self-assembled coatings on the metallic substrates. These coatings are a dense silicon and oxygen rich network and constitute a physical barrier that protects the metallic substrate form the aggressive environment.

Thus, the barrier properties of silane coatings are fundamental for improved corrosion protection and longer lifetime of the pre-treated substrates.

This work aims at developing and studying new pre-treatments for multi substrate applications based on functional silane coatings doped with corrosion inhibitors. The final goal is to enhance the barrier properties of the silane coating and, simultaneously, to make the coatings "smarter" in the presence of corrosion activity. This will be achieved by the release of inhibitor from the silane coating network during surface damage and corrosion activity.

The present work investigates the electrochemical behaviour of different substrates (galvanised steel, cold rolled steel, aluminium and magnesium alloys AZ31) pre-treated with different bis-functional silanes doped with cerium or lanthanum ions. The ability of the doped coating to mitigate corrosion was evaluated by electrochemical impedance spectroscopy (EIS) and by the scanning vibrating electrode technique (SVET).

The morphological characterisation of the doped coatings was performed by atomic force microscopy (AFM) and scanning electron microscopy (SEM).

The results showed that the Ce-doped coatings provide higher corrosion protection in all the substrates. The corrosion protection performance is dependent on the substrate, on the silane solution and on the dopant.

Publicado em:
Livro de abstracts, EUROCORR 2006, 25-28 Setembro, Maastricht, Holanda

THE ROLE OF THE SUBSTRATE ON THE CORROSION INHIBITION PERFORMANCE OF CERIUM IONS

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Publicado em:
Livro de abstracts, LATINCORR 2006, 21 a 26 Maio 2006, Fortaleza, Brasil

Cerium nitrate is known to act as corrosion inhibitor for several substrates. The corrosion inhibition mechanism seems to be dependent on a number of parameters, including the nature of the metallic substrate. The present study aims at investigating the role of cerium ions on the corrosion protection of different metallic substrates: galvanised steel, cold rolled steel and aluminium alloys (AA2024-T3) exposed to NaCl solutions containing cerium ions.

The electrochemical behaviour of the metallic substrates in the presence of cerium ions was evaluated by the scanning vibrating electrode technique (SVET), by potenciodynamic polarization curves and by electrochemical impedance spectroscopy (EIS) measurements. The results show that the cerium ions inhibit the corrosion processes. However, the inhibition performance is dependent on the substrate, being more reduced for cold rolled steel substrates.

Analytical characterisation of the metallic substrates by X-ray photoelectron spectroscopy (XPS) revealed the presence of a Ce-rich film on the surface. The XPS results reveal the presence of Ce^{3+} and Ce^{4+}, suggesting a two-steps inhibition mechanism.

CORROSION PERFORMANCE OF CERIUM DOPED SILANE PRÉ-TREATMENTS ON ALUMINIUM ALLOYS

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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. By this reason the search of alternative materials for chromate conversion coatings has been increasing in the recent years.

Different alternatives have been reported, based on non-toxic or low toxicity chemicals, aiming to obtain processes that confer to the treated surfaces properties identical to those obtained with chromates. Recent published work reported that silane treatments of metals before painting increase their corrosion performance.

The present work aims at the evaluation of the corrosion resistance of a pre-treatment based on bis-[triethoxysilylpropyl] tetrasulfide (BTESPT) doped with cerium nitrate on aluminium alloy substrates. Electrochemical impedance spectroscopy (EIS) and Scanning Vibrating Electrode Technique (SVET) were used to evaluate corrosion resistance during immersion in NaCl solutions. Atomic Force Microscopy (AFM) was used to characterize the morphology evolution of doped silane films. The results show that the pre-treatment provides very good corrosion protection to the substrates and that the doping with small amounts of cerium nitrate leads to a satisfactory inhibition effect. Furthermore, the results evidence improved protection comparatively to the pre-treatment only with BTESPT, both for Al 1050 and AA2024-T3.

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CUSTOMER SATISFACTION MEASUREMENT WITH DUMMY VARIABLE REGRESSION WITH CONSTRAINTS

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

A CRITICAL REVIEW OF CUSTOMER SATISFACTION MEASUREMENT IN TOURISM INDUSTRY

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This paper reviews and discusses the topic of customer satisfaction and its measurement. Defines the concept of customer satisfaction and some models used to access customer satisfaction in service and in particular in tourism industry. The paper highlights some tendencies of customer satisfaction measurement and makes a critical analysis of scales of measurement and its influence in data analysis techniques. The paper also focuses a methodology that can overcome problems of data analysis and concludes with some topics for future research in this subject.

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SYNTHESIS AND CHARACTERIZATION OF HYDROXYAPATITE

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Hydroxyapatite (HAP), is represented by the formula $Ca_{10}(PO_4)_6(OH)_2$, and is one of the inorganic components of the hard tissues of living bodies such as bones and teeth. HAP is a calcium phosphate based bio-ceramic, which has been used for several years in medicine and dentistry because of its excellent biocompatibility with human tissues. The success of its application in these fields depends upon factors such as the composition, crystallinity, size and morphology of HAP particles. This paper describes the work performed regarding the synthesis of this compound by a wet method comprising the direct precipitation of orthophosphoric acid solution to a calcium hydroxide solution, the process being described by the following reaction: 10 $Ca(OH)_2$ + 6 $H_3(PO_4)$ ‹=› $Ca_{10}(PO_4)_6(OH)_2$ + 18 H_2O. Synthesis was performed in a laboratory reactor, 700 mL in capacity, instrumented and controlled using a computer interface, so that the influence on process variables such as reaction temperature, pH, medium inertization by N_2, velocity of stirring and the flow rate input of $H_3(PO_4)$, could be assessed. The influence of these parameters was, therefore, evaluated in terms of the required composition and morphology of HAP formed particles, analysing them by FTIR, XRD, SEM and EPMA for determination of the Ca/P ratio. From the obtained results, it can be concluded that HAP particles having suitable properties for use in medicine, could effectively be prepared by this technique, provided that a good control of the involved process variables is maintained.
This preliminary work is part of a broader study aiming to the scale-up of the reactor.

"OPTIMIZATION OF SACCHARIDE FRACTIONATION USING NANOFILTRATION/ULTRAFILTRATION"

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Galacto-oligosaccharides (GOS) have limited digestibility, prebiotic properties and low-calorie sweetener potential. Therefore, are dietary food ingredients with a significant world annual production (over 15,000 t/yr). GOS are produced from the lactose — present in second cheese whey — using enzyme reactors (with b-galactosidases). Short residence times in a continuous bioreactor allow higher GOS concentration in the outflow, unfortunately together with the unreacted substrate. This means that to obtain a better industrial product it is very important to develop processes able to fractionate such a stream in mono-/di- and tri-/oligosaccharides. Then, unreacted lactose could be recycled to the enzyme reactor. Nanofiltration (NF) has a high potential for industrial application in a GOS production process as it is reliable and simple to scale-up. The fractionation of saccharides and oligosaccharides by nanofiltration depends on: membrane pore size distribution [1], solutes concentration and pH. This work investigates the dependence of the fractionation of low molecular weight model-saccharide mixtures on the membrane molecular weight cut-off (MWCO) and on the solute concentration. The model saccharides tested were glucose, sucrose, lactose, raffinose and melezitose.

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Euromembrane 2006, Giardini Naxos, Taormina (Messina), Italy, 24-28 de Setembro, 2006

"REDUCTION OF WASTEWATERS AND VALORISATION OF BY-PRODUCTS FROM "SERPA" CHEESE MANUFACTURE USING ULTRAFILTRATION AND NANOFILTRATION"

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Second cheese whey (SCW) is a by-product of cheese and curd cheese production that is usually not recovered and therefore substantially contributes for the negative environmental impact of the cheese manufacture plants. Membrane technology, namely nanofiltration (NF), is used in this work for the recovery of SCW organic nutrients, resulting from "Serpa" cheese and curd production. The SCW is processed by nanofiltration to recover a rich lactose fraction in the concentrate and a process water with a high salt content in the permeate.

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

"O DESAFIO DE TECNOLOGIAS EMERGENTES NUMA PERSPECTIVA AMBIENTAL INTEGRADA"

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No início da segunda metade do século XX a inovação industrial significava o desenvolvimento de novos processos/produtos na óptica de uma sociedade de consumo baseada na utilização de matérias-primas abundantes e baratas e recursos hídricos e energéticos ilimitados. A alteração desta situação, escassez e degradação dos recursos naturais, coloca o desafio de aplicação de tecnologias emergentes em combinação com tecnologias convencionais conducentes a um desenvolvimento sustentável em que os novos processos são caracterizados por uma produção mais eficiente e selectiva com redução do consumo de recursos, minimização de resíduos e sua potencial reutilização/valorização como novos produtos.

As estratégias de recuperação de águas residuais, com o objectivo da implementação de ciclos fechados de água na indústria , da recuperação de componentes com potencial de valorização, requerem, na maior parte do casos, uma combinação de diferentes processos unitários de tratamento que devem ser seleccionados de acordo com os usos e sem comprometer a viabilidade técnico-económica dos processos produtivos.

A demonstração desta abordagem sistemática será apresentada em quatro casos industriais – Lacticínios, Cartão Canelado/Embalagem, Coqueria e Cortiça.

Apresentado em:
Simpósio – "A investigação na Universidade Técnica de Lisboa", Lisboa, Portugal, 2 e 3 de Fevereiro de 2006

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

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Apresentado em:
ENVENT – Encontro Nacional de Ventilação, Espinho, 12 e 13 de Julho de 2006

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

"QUALIDADE DO AR INTERIOR EM EDIFÍCIOS"

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Estudos realizados sobre a natureza e extensão da poluição do ar revelaram que a qualidade do ar interior é a parte mais significativa da exposição pública à poluição do ar. É um dado adquirido que a exposição das populações ao ar interior varia significativamente dependendo das condições climáticas, estilos de vida, hábitos culturais, etc. Em geral, em meios urbanos, esta exposição excede 90% (60% no local de residência, 30% no local de trabalho e 5% no tráfego urbano). Estas razões levaram ao aparecimento do Síndroma do Edifício Doente que afecta cada vez mais indivíduos e que ocorrem frequentemente em edifícios novos com sistema central de ventilação em que o tipo de sistema de humidificação resulta em fonte de contaminação por micróbios e fungos e a luz artificial fluorescente é uma fonte potencial de smog fotoquímico. Este síndroma apresenta várias vertentes como sejam a exposição dos indivíduos a níveis elevados de poeiras no ar e de compostos orgânicos voláteis libertados pelos materiais de construção e infiltrados a partir do exterior além das doenças provocadas por vírus e bactérias resultantes da má manutenção e limpeza dos sistemas de ar condicionado dos quais a legionella é, presentemente, aquela que resulta em consequências mais graves como sejam as infecções pulmonares e as pneumonias. Por todas estas razões urge realizar, sistematicamente, a verificação do projecto do sistema de ventilação e condicionamento térmico em edifícios e a monitorização dessas mesmas condições nos edifícios já construídos, como se encontra especificado pela recente legislação nacional (Decreto-lei Nº 78/2006 de 4/04).

Apresentado em:
Dias do Departamento de Engenharia e Ciências Naturais da ULHT, Lisboa, Novembro de 2006

"ASPECTOS ECONÓMICOS DO CONTROLO DOS EFLUENTES GASOSOS"

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Apresentado em:
Seminário sobre Controlo das Emissões Gasosas, Lisboa, 26 de Outubro de 2006

Recentemente a Comissão Europeia levou a cabo estudos para estimar os benefícios monetários de propostas para melhorar a qualidade do ar e reduzir impactos ambientais negativos. Os estudos realizados anteriormente sugeriram que se poderiam obter elevados benefícios monetários, mesmo a partir de pequenas melhorias na qualidade do ar. Naturalmente que isto provocou um aceso debate entre aqueles que queriam acreditar nessas conclusões e aqueles que reputaram essas estimativas como demasiado elevadas. Esta continua a ser uma área de estimativa muito difícil, mas verificou-se recentemente, uma mudança de opinião a favor de estimativas mais conservadoras. Tipicamente, os benefícios monetários da melhoria da qualidade do ar podem resultar dos seguintes factores: Redução dos impactos negativos sobre a saúde humana (no curto e longo prazo); Redução dos impactos negativos sobre as culturas e ecossistemas; Redução do desgaste dos materiais, edifícios e monumentos; Melhoria da visibilidade, pela redução das substâncias que provocam névoas fotoquímicas.

Não existem até agora, métodos monetários satisfatórios para avaliar dos benefícios para os ecossistemas; O que é lamentável do ponto de vista cientifico e fornece argumentos a quem afirma que as estimativas actuais apresentam valores por defeito. Este é um aspecto que não pode continuar a ser desprezado no futuro, pelo que deverá ser dedicada mais atenção ao desenvolvimento de modelos nesta área. Os estudos levados a cabo pela Comissão Europeia reflectiram já alguns avanços sobre este aspecto particular ao considerarem um sistema de classificação que relaciona as avaliações monetárias aplicáveis a cada um dos impactes. Esta classificação considera, separadamente a inclusão e a não inclusão dos factores que são, hoje mais afectados pela incerteza da estimativa. Contudo, é desejável que estas classificações incluam não só, a incerteza associada ao valor monetário atribuído a cada benefício, mas também à probabilidade de que um determinado poluente seja, de facto a causa de um dado efeito e ainda que esse efeito se verifique para as concentrações ambientais em questão. De facto, as maiores fontes de incerteza são:

a utilização de projecções relativas a emissões, modelações, cálculo de exposição número de pessoas afectadas, resposta das plantas à concentração de determinados poluentes que reduzem a concentração da camada ozono protectora e a significância dos danos sobre os ecossistemas.

Contudo, há mais factores a serem considerados: o custo do controlo das emissões gasosas são geralmente calculados numa base muito diferente das estimativas dos benefícios monetários, que é o gasto real com as tecnologias de controlo de emissões. Por outro lado, muitas das estimativas dos benefícios monetários são baseados no valor que o público "está disposto a pagar". Isto aponta para que estas duas abordagens não são, de todo, comparáveis e não é lícito fazer estimativas considerando, simultaneamente factores obtidos através destas diferentes abordagens. Em conclusão, pode dizer-se que, para uma aplicação correcta destas estimativas há ainda muitos aspectos que têm que ser definidos e classificados, pelo que é urgente proceder à realização de estudos adicionais sobre esta área. Outras questões relacionam-se com a responsabilidade da sociedade em geral e dos governos em particular, assim como do uso eficiente e económico de recursos finitos.

Assim, será importante saber se a redução dos riscos resultantes da alocação de recursos escassos para reduzir as emissões de um poluente em particular vale mais do que o benefício social que pode ser retirado de se aplicarem esses mesmos recursos para outro fim; ou seja, haverá outras formas economicamente mais adequadas de melhorar a saúde humana e a qualidade de vida da população em geral, em vez da redução da poluição do ar?

VARIATION OF DIMENSIONAL STABILITY AND DURABILITY OF EUCALYPT WOOD BY HEAT TREATMENT

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Eucalypt (*Eucalyptus globulus Labill.*) wood, a non durable species with low dimensional stability, is used in Europe almost exclusively for pulp and paper or as firewood. Heat treatment is an ecological way to improve the dimensional stability and durability of wood without the use of harmful chemicals.

Eucalypt wood was tested with two kinds of heat treatment: (a) in an oven in the presence of air for 2 to 24 h at 170-200 ºC and (b) in an autoclave in the absence of air with superheated steam for 2 to 12 hours at 190- 210 ºC. Equilibrium moisture content, dimensional stability (measured as ASE, anti shrinkage efficiency), modulus of elasticity (MOE), bending strength, wettability and resistance against fungus (Trametes versicolor (L.exFt.) Pilat) and termites (Reticulitermes grassei Clément) were determined.

The equilibrium moisture content of the heat treated eucalypt wood decreased by 68% and 61% respectively for oven and autoclave treatment, respectively. The dimensional stability in radial direction, measured at 65% air relative humidity (ASE65), increased with temperature and treatment time, and more for the oven-heat-treated wood, reaching 73% and 72%, respectively. Wettability of the heat treated wood decreased for both treatments. Bending strength and MOE decreased for both heat treatments, respectively by 60% and 15-25%. At the same mass loss the decrease was higher for oven heat treated wood. Fungal durability against Trametes versicolor improved with both treatments but the resistance against termite attack was similar for treated and untreated wood.

The heat treatment improved the behaviour of eucalypt wood in relation to moisture and fungal attack and showed its potential for solid timber products.

SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF PIGMENTS FROM BIXA ORELLANA SEEDS: EXPERIMENTS AND MODELLING

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Supercritical CO_2 extraction of the pigments from Bixa orellana seeds was carried out in a flow apparatus at a pressure of 200 bar and a temperature of 40 ºC at two fluid flow rates (0.67g/min and 1.12g/min). The efficiency of the extraction was low (only about 1% of the pigment was extracted). The increase in flow rate led to a decrease in pigment recovery. A large increase in recovery (from 1% to 45%) was achieved using supercritical carbon dioxide with 5 mol % ethanol as extraction fluid at pressures of 200 and 300 bar and temperatures of 40 and 60 ºC. Although the increase in temperature and pressure led to an increase in recovery, the changes in flow rate did not seem to affect it. Furthermore, two plug flow models were applied to describe the supercritical extraction of the pigments from annatto seeds. Mass transfer coefficients were determined and compared well with those obtained by other researchers with similar models for the supercritical extraction of solutes from plant materials.

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DENSITY MEASUREMENTS OF FLUIDS AND THEIR MIXTURES AT HIGH PRESSURE

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\Proceedings of 3rd International Meeting High Pressure Chemical Engineering, Erlange, Germany Engineering, Copenhagen, 2006, pp. 1-6.

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

ENZYMIC REACTIONS IN SUPERCRITICAL CARBON DIOXIDE

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Glucose 2-oxidase (pyranose oxidase, pyranose:oxygen-2-oxidoreductase, EC 1.1.3.10) from Coriolus versicolor catalyses the oxidation of D-.glucose at carbon 2 in the presence of molecular oxygen producing D-glucosone (2-keto-glucose and D-arabino-2-hexosulose) and hydrogen peroxide. This enzyme was used to convert D-glucose into D-glucosone at high pressures with compressed air in a modified commercial batch reactor. Several parameters affecting biocatalysis at high pressures were investigated as follows: pressure, enzyme concentration, glucose concentration, supercritical fluid and the presence of catalase. Glucose 2-oxidase was purified by immobilized metal affinity chromatography on epoxy-activated Sepharose 6B-IDA-Cu(II) column at pH 6.0. The conversion of D-glucose into D-glucosone was dependent on the pressure since an increase in the pressure with compressed air resulted in higher rates of conversion. On the other hand, the presence of catalase increased the rate of reaction which strongly suggests that hydrogen peroxide inhibited the rate of reaction. The rate of conversion of D-glucose into D- glucosone by glucose 2-oxidase in the presence of either nitrogen or supercritical CO_2 at 110 bar was very low compared with the use of compressed air at the same pressure.

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Livro de abstracts of COST ACTION D30-Kick Meeting WG D30/008/06, Prague, Czech Republic, (2006).

FENOMENOLOGIA DA COMBUSTÃO E EXTINTORES

Guerra, A.M.; Coelho, J.A.; Leitão, R.E.

Publicado em:
Escola Nacional de Bombeiros, ISBN: 972-8792-23-9, Janeiro 2006, 2ªEd., pg. 1-104.

A fenomenologia da combustão e extintores aborda um tema de primordial importância para a formação de base do bombeiro. A correcta compreensão e aquisição de conhecimentos expostos neste volume, de uma forma simples, permitirá uma mais valia para qualquer bombeiro que posteriormente deverá desenvolver e aperfeiçoar.

Para se entender o fenómeno do fogo, como reacção química particular acompanhada pela libertação de calor, é necessário conhecer a natureza da matéria, assim como, a sua constituição de base. A matéria e as suas formas de ligação encontram-se intimidando relacionadas com o seu estado físico e, consequentemente, às características do combustível e do comburente. A conjunção destes dois factores com a energia de activação e a reacção em cadeia, permitem desenvolver uma série de considerações, normalizações e definições, fundamentais para o entendimento deste fenómeno.

A classificação, características e funcionamento dos extintores é uma das contribuições importantes para este volume, que, de uma forma directa ou indirecta, se encontram relacionados com o estado físico do agente extintor e aspectos físico-químicos dos mesmos. Neste volume estes conceitos básicos são apresentados ao longo do texto, pretendendo-se realçar aspectos mais importantes, assim como, a utilização das actuais normas europeias e portuguesas.

DESENVOLVIMENTO DE UM BIOSSENSOR POTENCIOÉTRICO PARA ACRILAMIDA USANDA AMIDASE SELVAGEM DE Pseudomonas aeruginosa

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Mestrado em: Biofísica (Especialização em Biofísica e Física Médica)
Grau Concedido por: Faculdade de Ciências da Universidade de Lisboa
Orientador e Co-orientador: Professor Doutor Amin Karmali e Porfessor Doutor Eduardo Ducla Soares
Provas Concluídas em: 7 de Fevereiro de 2006

Esta dissertação desreve o desenvolvimento de um biossensor potenciométrico para a determinação de acrilamida, utilizando como elemento bioactivo a amidase selvagem de *Pseudomonas aeruginosa*.
A importância da determinação de acrilamida é reconhecida mundialmente. As eventuais consequências são a mutagenicidade, carcinogenicidade e neurotoxicidade. Deve ser considerado o interesse nas áreas ambiental, ambiental e clínica, já que a acrilamida pode ter acções diferentes dependendo da sua concentração. Devido à complexidade das amostras e à baixa concentração do analito em análises ambiental, alimentar e clínica, os biossensores destacam-se como um sistema de detecção potencialmente sensível, selectivo, rápido e barato. Os objectivos específicos deste trabalho foram: (i) produção e purificação da amidase selvagem de *Pseudomonas aeruginosa*; (ii) imobilização das moléculas de amidase covalentemente à superfície activada de uma menbrana de polietersulfona na presença do agente bifuncional glutaraldeído; (iii) construção do eléctrodo enzimático, através do acoplamento da membrana imobilizada directamente na base de um ISE de amónio; (iv) optimização da resposta potenciométrica através do estudo de parâmetros que afectam a actividade enzimática (tempo de imobilização, concentração de glutaraldeído, concentração de enzima, pH da mistura reaccional) e (v) estudo das características analíticas do biossensor (gama linear de resposta, sensibilidade, limite de detecção, tempo de resposta e estabilidade).
A acrilamida, na presença de amidase foi enzimaticamente transformada em iões amónio, os quais foram monitorizados potenciometricamente através da utilização de um eléctrodo selectivo a iões amónio. Nas condições óptimas encontradas, a relação entre a resposta potenciométrica e o log[acrilamida] foi linear entre 0,02 e 0,28 mM, a sensibilidade foi de 52,5 mV/década, o tempo de resposta $t_{90\%}$ foi de 36s e foi alcançada uma estabilidade, trauzida como tempo de meia vida ($t_{1/2}$) de 24 dias. Estes dados sugerem aparentemente que o biossensor poderá ser usado para a determinação de acrilamida em amostras biológicas e não biológicas.

QUÍMICA DE COORDENAÇÃO DE ESCORPIONATOS E OUTROS LIGANDOS INSATURADOS DE AZOTO EM CENTROS DE RÉNIO, MOLIBDÉNIO OU FERRO

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Provas Concluídas em: 16 de Junho de 2006

Desde o trabalho pioneiro de Trofimenko, os complexos com ligandos aniónicos azotados, tridentados tris(pirazolil)boratos [$HB(pz)_3$, abrev. Tp] e relacionados como por exemplo o tris(3,5-dimetilpirazolilborato) [$B(Me_2pz)_3$, abrev. Tp^{Me}] também conhecidos por "ligandos escorpionatos", têm despertado grande interesse devido às suas aplicações na área da catálise, síntese inorgânica, bioinorgânica e organometálica. Neste trabalho de doutoramento é descrita a síntese e caracterização dos seguintes novos compostos de rénio ou de ferro com ligandos azotados de tipo tris(pirazolil)metano ou derivados pirazoles: com hidrotris(1-pirazolil)metano $[ReCl_2\{k^3\text{-}HC(pz)_3\}(PPh_3)][BF_4]$, $[ReCl_3\{k_3\text{-}HC(pz)_3\}]$, $[ReCl_4\{k^2\text{-}HC(pz)_3\}]$, $[FeCl_2\{k^3\text{-}HC(pz)_3\}]$, hidrotris(3,5-dimetil-1-pirazolil)metano $[ReCl_2\{k^3\text{-}HC(3,5\text{-}Me_2pz)_3\}(PPh_3)][BF_4]$, $[ReCl_3\{k^3\text{-}HC(3,5\text{-}Me_2pz)_3\}]$, tris(pirazolil)metanossulfonato, $[ReOCl\{k^3\text{-}SO_3C(pz)_3)(PPh_3)]Cl$, $[ReO_3\{k^3\text{-}SO_3C(pz)_3)]$, $[ReO\{SO_3C(pz)_3\}\{OC(CH_3)_2(pz)\}][ReO_4]$, $Li[FeCl_2\{k^3\text{-}SO_3C(pz)_3)]$, pirazole $[ReCl_2\{N_2C(O)Ph\}(Hpz)(PPh_3)_2]$, $[ReCl_2\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$, $[ReClF\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ e 3,5-dimetilpirazole $[ReCl_2(3,5\text{-}Me_2Hpz)_3(PPh_3)]Cl$.
Investigou-se a actividade catalítica de alguns destes compostos na oxidação do etano a ácido acético, num só "passo", e na oxidação peroxidativa do ciclo-hexano, originando ciclo-hexanona e ciclo-hexanol, em condições suaves. É ainda, apresentada a síntese e caracterização de vários compostos de cianoimido, derivados de (i) alquilação, *trans*-$[Mo(NCN)(NCNR)(dppe)_2]X$ (R = Me, X = I; R = Et, X = I; R = Pr, X = I; R = $CH(CH_3)_2$, X = I; R = $CH_2C_6H_5$, X= Br; R = $CH_2C_6H_4NO_2$, X = Br, R = Me, X = BF_4), (ii) acilação, *trans*-$[Mo(NCN)\{NCNC(O)R\}(dppe)_2]Cl$ (R = Me), e reacções subsequentes com electrófilos e nucleófilos.
O comportamento electroquímico dos compostos sintetizados foi estudado por voltametria cíclica ou electrólise a potencial controlado. Por simulação digital de voltametria cíclica (VC) estabeleceu-se o mecanismo da isomerização *trans-cis* electroinduzida observada nos compostos *trans*-$[Mo(NCN)\{NCNC(O)R\}(dppe)_2]Cl$ (R = Me, Et ou Ph). Foram estimados os valores do parâmetro electroquímico E_L dos ligandos N_2COPh, $HC(pz)_3$, $3,5\text{-}Me_2Hpz$, $HC(3,5\text{-}Me_2pz)_3$ e $SO_3C(pz)_3^-$ permitindo assim avaliar e comparar o carácter doador/aceitador.

CONTRIBUTO PARA O ESTUDO DAS TRANSFORMAÇÕES DO AZOTO NO PROCESSO DE COMPOSTAGEM DE LAMAS DE AGRO-INDÚSTRIAS

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O estado da arte sobre a compostagem de resíduos orgânicos aponta as perdas de azoto por volatilização como um dos problemas da condução do processo, que não só reduzem o poder fertilizante do produto final, como também são responsáveis pelos odores indesejáveis. Essas perdas estão directamente relacionadas com a dinâmica do azoto no processo principalmente com os parâmetros que influenciam o equilíbrio das formas amoniacais.
O presente trabalho teve como objectivos avaliar as potencialidades da aplicação do processo de compostagem para estabilização das lamas produzidas no tratamento de efluentes de uma indústria de processamento e transformação de carne avícola e quantificar as perdas de azoto por volatilização. Procurou-se com este trabalho abordar o problema de tratamento deste tipo de resíduos de uma forma prática e exequível e, como consequência, a escolha das misturas estudadas não foi indiferente a questões relacionadas com a disponibilidade de materiais, operacionalidade e custos envolvidos.
O plano experimental compreendeu duas fases, que incluíram ensaios laboratoriais de simulação das condições de compostagem em reactor *batch*, com temperatura e arejamento controlado. Na primeira fase, foi avaliada a diferença de biodegradabilidade para várias misturas possíveis de efectuar à escala real no tratamento por compostagem destes resíduos. Na segunda fase, acompanharam-se as transformações do azoto e foram quantificadas as perdas de azoto por volatilização para diferentes misturas.
Os resultados obtidos permitiram concluir que a estabilização deste tipo de lamas pode ser conseguida através do processo de compostagem, numa perspectiva de reaproveitamento e reciclagem de nutrientes. Verificou-se que o pó de madeira, escolhido como fonte de carbono, não foi utilizado pelos microrganismos no tratamento de lamas primárias enquanto que no tratamento de lamas secundárias foi utilizado no processo biológico. Por outro lado, a casca de arroz mostrou ser um agente adequado para conferir a estrutura necessária e melhorar as propriedades físicas das lamas. Verificou-se ainda que, as perdas de azoto por volatilização estão directamente relacionadas com a actividade microbiológica e que o aumento da relação C/N conduziu a menores perdas de azoto por volatilização.

WILD-TYPE AND RECOMBINANT MUTANT AMIDASES FROM PSEUDOMONAS AERUGINOSA: STRUCTURAL AND KINETIC CHARACTERIZATION BY USING MONOCLONAL ANTIBODIES

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Amidase (acylamide amidohydrolase; E.C. 3.5.1.4) catalyses the hydrolysis of aliphatic amides producing the corresponding acid and ammonia. Therefore, a novel assay method using an ammonium ion-selective electrode (ISE) was investigated. Kinetic properties of wild-type and recombinant mutant amidases were studied and the results obtained by using this real time assay method were in agreement with the linked assay method. Additionally, the effect of hydroxylamine on amidases activities was studied. Hydroxylamine was found to act as an activator of the hydrolysis of amides catalysed by wild-type and mutant (T103I, W138G and C91A) amidases. Since wild-type and mutant T103I amidases exhibit different substrate specificities, monoclonal antibodies (MAbs) were raised against these enzymes by hybridoma technology, in order to study structural changes on amidase molecule. Some polyol-responsive MAbs (PR-MAb), were identified by ELISA elution assay and MAbs of IgM (E2A6) and IgG (C9E4) classes recognized specifically a common epitope on wild-type and mutant (T103I) amidases. MAb E2A6 exhibited higher affinity for denatured enzymatic forms than for native forms, suggesting that it recognizes a cryptic epitope on amidase molecule. MAb C9E4 appears to bind to a conformation-sensitive epitope, since it did not recognize denaturated wild-type and mutant T103I amidases. Furthermore, MAb C9E4 did not recognize native and denaturated forms of recombinant mutant C91A amidase suggesting that this substitution disrupted the conformational epitope. These MAbs are useful probes to differentiate wild-type and mutant (T103I and C91A) amidases since they also affect differently their enzyme activity.
MAbs from IgM (E2A6) and IgG (C9E4) classes were also purified by metal ion affinity chromatography (IMAC). The adsorption of MAbs onto immobilized metal chelates was due to coordination of histidine residues available in the 3rd constant domain of heavy chain (CH3) of immunoglobulins. The effect of ligand concentration, the length of spacer arm and the nature of metal ion were studied. Culture supernatants containing MAbs of IgM and IgG classes were purified by IMAC on EPI-60-IDA-Co(II) and commercial IDA-Zn(II) columns at pH 8.0 with a specific content of 0.78 and 1.0 mg Ig.mg-1 protein and a purification factor of 19.5 and 20, respectively.

ESTUDO DE FILMES DE BIS-[TRIETOXISILIL]TETRASULFANO (BTESPT) PARA PRÉ-TRATAMENTOS ANTICORROSIVOS DA LIGA DE ALUMÍNIO 2024-T3

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Provas Concluídas em: 10 de Julho de 2006

A necessidade de substituir os pré-tratamentos à base de cromatos, utilizados na indústria de tratamento de superfícies metálicas, tem impulsionado, nos últimos anos uma busca intensiva de tecnologias alternativas. De entre as alternativas viáveis, os silanos apresentam bom desempenho, são de fácil aplicação e podem ser aplicados numa vasta gama de substratos metálicos.
Este trabalho teve por objectivo o estudo do comportamento anticorrosivo e a caracterização analítica e estrutural de um pré-tratamento à base de silano (BTESPT) aplicado na liga de alumínio 2024-T3. Os filmes obtidos foram caracterizados por elipsometria, Auger/XPS, AFM, SEM/EDS, SKPFM, SVET e EIS.
Os resultados mostraram que se forma, na superfície da liga, um filme que revela boas propriedades anticorrosivas. No entanto, estes filmes não apresentam o efeito de auto reparação típico dos filmes à base de cromatos, não podendo assim assegurar uma protecção anticorrosiva activa. A adição de uma pequena quantidade de nitrato de cério à solução de silanos, permitiu obter filmes com melhores propriedades anticorrosivas, que parecem revelar capacidade de auto reparação, tornando-se esta alternativa promissora, no que se refere à substituição dos tratamentos com cromatos.


05

ENGENHARIA DE SISTEMAS DE POTÊNCIA E AUTOMAÇÃO

Anuário Científico 2006

ISEL

CONTROLO DE UM MANIPULADOR ROBÓTICO USANDO VISÃO

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Este trabalho descreve uma metodologia que permite que um manipulador, equipado com uma câmara de vídeo, se aproxime de um objecto a manipular. A principal característica é que para tal não vamos recorrer a informação de calibração da câmara, o que permite uma grande flexibilidade. O manipulador é controlado unicamente pela informação que retira da imagem, não necessitando inverter a cinemática do sistema. A única restrição é a necessidade de o objecto a capturar estar localizado num plano. Utiliza-se uma rede neuronal na cadeia de controlo, que calcula uma aproximação do jacobiano inverso, não se procedendo, deste modo, à pré-calibração do sistema e não é necessário conhecer as características do manipulador ou do sistema de visão.

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05

PARAMETERISATION EFFECT ON THE BEHAVIOUR OF A HEAD DEPENDENT HYDRO CHAIN USING A NONLINEAR MODEL

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This paper is on the problem of short-term hydro scheduling (STHS), particularly concerning a head-dependent hydro chain. We use a method based on nonlinear programming (NLP), namely quadratic programming, to consider hydroelectric power generation a function of water discharge and of the head. As a new contribution to earlier studies, which presented reservoir operation rules mainly for medium and long-term planning procedures, we show that the physical data defining hydro chain parameters used in the nonlinear model have an effect on the STHS, implying different optimal storage trajectories for the reservoirs accordingly not only with their position in the hydro chain but also with the new parameterisation defining the data for the hydro system. Moreover, considering head dependency in the hydroelectric power generation, usually neglected for hydro plants with a large storage capacity, provides a better short-term management of the conversion of the potential energy available in the reservoirs into electric energy, which represents a major advantage for the hydroelectric utilities in a competitive electricity market. We conclude as the main contribution of this paper for the short-term management of head-dependent hydro chains that there is no clear and definitive rule about what is the volume of the water to store in each reservoir at each period to achieve the optimum STHS based only on the reservoirs relative position.

NOVEL LINEARIZATION TECHNIQUE FOR LOW-DISTORTION HIGH-SWING CMOS SWITCHES WITH IMPROVED RELIABILITY

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High-linearity switches are required in many low-voltage switched-capacitor (SC) circuits, spanning from 10-14b ADCs to accurate analog filters. As CMOS technologies continue to evolve towards lower supply voltages, new design techniques are needed to provide analog switches capable of rail-to-rail swings while exhibiting low-distortion. Furthermore, when requiring low-voltage operation, the reliability constraints of the technology have to be considered, avoiding over-stress of the CMOS devices due to large voltages being applied to the transistor gate. This paper proposes a linearization technique for low-distortion high-swing CMOS switches based on a new method of improving the linearity of the NMOS and PMOS conductances. This method has the advantage over conventional clock-boosting techniques of avoiding large gate voltages thus reducing the stress on the gate capacitance. Simulated results of a practical sample-and-hold circuit show that, using this technique, linearity levels compatible with 12-b can be reached over the Nyquist band.

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Proc. IEEE ISCAS'06, pp. 2001-2004, Kos, Greece, May 2006.

SHORT-TERM WIND SPEED PREDICTION AND WIND POWER GENERATION OUTPUT

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Proc. of 2nd International Conference on Knowledge Engineering and Decision Support (ICKEDS'06). ISBN: 972-8688-39-3. Lisboa, Portugal, Maio de 2006

Portugal is increasing the power capacity in renewable resources, to reduce the dependence on fossil fuels, expecting in 2010 to achieve 3750 MW of installed power capacity in wind generators. This important installed power capacity may cause problems to the operation of the electrical grid because wind power follows wind speed fluctuations. Due to this direct dependence it is important to forecasts the wind speed for several spears. In this work the wind speed of one hour ahead forecast is addressed, using neural networks of Multi Layer Perceptrons with backpropagation learning algorithm. The values to wind speed forecast are chosen, the learning patterns of the neural network are created and the learning strategies are defined by choosing the neural network architectures and the number of iterations. Several tests are performed with various neural network architectures and several data sets, allowing the choice of the network that presents the best generalization. The results are compared with other short-term forecast methods usually considered as reference.

PREVISÃO DE POTÊNCIA EÓLICA USANDO REDES NEURONAIS ARTIFICIAIS

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Portugal pretende aumentar a potência instalada em centrais que utilizam recursos renováveis, de modo a reduzir a dependência dos combustíveis fósseis e a quantidade de emissões de gases de efeito de estufa, objectivando atingir em 2010, 3750 MW de potência instalada em geradores eólicos. Sendo o vento um recurso impossível de controlar poderão ocorrer problemas na gestão da produção. As redes neuronais artificiais têm demonstrado elevadas performances em problemas de previsão. Neste trabalho foram usadas redes feedforward de perceptrões multicamada treinadas com um algoritmo de retropropagação dos erros. Foram feitos vários ensaios com o intuito de escolher a arquitectura da rede que apresenta a melhor generalização. Adicionalmente, foram feitas várias previsões da velocidade do vento e comparadas com alguns métodos considerados de referência. Estes valores previstos foram aplicados a um gerador eólico e avaliados os seus resultados.

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Actas do IST Fórum Energia – Primavera 06, Volume 2 nº 01. IST, Portugal, J18 de Maio de 2006, Pág.58-61

MEASURING MARKET POWER IN THE SPANISH ELECTRICITY MARKET USING A CONJECTURAL VARIATIONS APPROACH

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Proceedings da 3ª conferência The European Electricity Markets – Challenge of the Unification, Varsóvia, Polónia, Maio de 2006.

In electricity markets the strategic behaviour of supply side market participants is the major driver for the day-ahead market clearing price. This individual strategic behaviour of market participants can be derived from the estimate of their values of conjectural variations.
In this paper we present a conjectural variations approach to estimate de degree of competitiveness of the four major generating companies (Endesa, Iberdrola, Unión Fenosa and Hidrocantábrico) that operate in the Spanish electricity market, for the period from January 2004 to November 2005.
The results achieved show that these companies had changed their strategic behaviour on 2005 in comparison to 2004, what might have been one of the causes of the increase in the electricity market clearing prices observed in the Spanish pool during the year of 2005.

THE FUTURE IBERIAN ELECTRICITY MARKET IMPACT ON THE PORTUGUESE AND SPANISH POWER PRODUCERS USING A CONJECTURAL VARIATIONS MODEL

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The impact of the future Iberian Electricity Market (IBELM) is a major concern for the Iberian power producers and consumers, since price reductions due to increasing competition will favour consumers and harm producers for unchanging quantities sold.
In this regard, it is presented in this paper an evaluation of the impact of the IBELM on power producers. For that purpose a conjectural variations model is implemented in GAMS, where different competitive regimes were considered, ranging from perfect competition to collusive arrangements. Simulations were carried out for the Portuguese and Spanish markets in autarky and integrated in the IBELM.
Conclusions are presented in respect to the IBELM impact on the market clearing price, as well as on power generation and profits of the Portuguese and Spanish power producers EDP, Tejo Energia, Turbogás, Endesa, Iberdrola, Unión Fenosa and Hidrocantábrico.

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Proceedings da 3ª conferência The European Electricity Markets – Challenge of the Unification, Varsóvia, Polónia, Maio de 2006.

STRATEGIC BIDDING ANALYSIS IN THE SPANISH ELECTRICITY MARKET USING A CLUSTER APPROACH

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Publicado em:
Proceedings da 3ª conferência The European Electricity Markets – Challenge of the Unification, Varsóvia, Polónia, Maio de 2006.

In order to fulfil power company's short term economic expectations, related to maximum production capacity, long-term decisions and market share, day-ahead bid curves work as the primary tool to reflect the strategic position of a player in a liberalised electricity market. Understanding the impact that price resources and other direct and indirect variables have on a company's rival's strategic bids is an undeniable advantage to predict immediate market behaviour. In this paper we address this issue with some considerations of the strategic bid curves used by the major players that operate in the Spanish electricity market. A cluster approach is used to identify the most relevant bid strategies of the players and the adequacy of the methodology for price forecasting is evaluated. The monthly price simulation examples, based on determined representative curves, lead to promising results.

EMISSIONS TRADING IMPACT ON THE IBERIAN ELECTRICITY MARKET

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The purpose of this paper is to evaluate the impact of the CO_2 emissions trading on the IBELM (Iberian Electricity Market), regarding complex aspects of the Spanish market such as the stranded costs CTC (Competition Transition Charges), which have a major impact on the power producer's strategies. For this purpose, a SIMulator for Electricity and Carbon markets (SIMEC, version 2.0) was developed in GAMS, which includes the modelling of the CTC's mechanism, the strategic interaction among companies, using game theory, and a CO_2 bidding strategy. Given the system power plants characteristics, demand data and CTC's amounts, SIMEC computes electricity market clearing price, power generation and CO_2 emissions by power plant, as well as power industry profits, for a range of CO_2 prices simulated within 0 and 40 /ton.

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MONITORIZAÇÃO E MODELAÇÃO DO COMPORTAMENTO DINÂMICO DE BARRAGENS DE BETÃO

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Neste trabalho pretende-se mostrar que os recentes desenvolvimentos ao nível dos equipamentos de medição de vibrações e ao nível das metodologias de identificação modal, possibilitam o desenvolvimento de sistemas de monitorização dinâmica para grandes barragens, que permitirão registar e analisar continuamente, com uma precisão aceitável, a resposta dinâmica destas obras sob a acção do ruído ambiente e sob acções sísmicas de diferentes intensidades. Salienta-se que, no âmbito das actividades de controlo da segurança de barragens, estes sistemas poderão ter grande interesse, nomeadamente: i) na análise de processos de deterioração evolutiva; e ii) na análise dos efeitos das acções sísmicas. Apresentam-se resultados de medições dinâmicas efectuadas na barragem do Cabril, sob a acção da excitação ambiente, os quais são comparados com resultados de anteriores medições realizadas em ensaios de vibração forçada. Os resultados observados são comparados com os de um modelo numérico de elementos finitos tridimensionais baseado na hipótese de comportamento elástico linear admitindo que o efeito hidrodinâmico da água é adequadamente simulado através de massas de água associadas segundo a fórmula de Westergaard.

PLANIFICACIÓN DE LA OPERACIÓN DE CORTO PLAZO DE SISTEMAS DE ENERGÍA HIDROELÉCTRICA

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La industria de los sistemas de energía eléctrica sufrió en las últimas décadas transformaciones sin precedentes. Para hacer frente a la competencia, las compañías tienen hoy que ver sus inversiones con más racionalidad, mediante la maximización del uso de los recursos que disponen y la minimización de los proyectos que no tengan una contribución directa para mejorar la racionalidad económica en la producción de energía eléctrica.

La planificación de la operación de sistemas de energía hidroeléctricos, teniendo en cuenta la disponibilidad de agua y las restricciones físicas y operacionales existentes, tiene como objetivo la maximización del valor de la producción hidroeléctrica total en el horizonte temporal considerado.

En este artículo se centra el estudio al corto plazo, es decir, desde un día hasta una semana, con periodos horarios, por lo que se pueden considerar las variables de naturaleza no estocástica. En la formulación del problema se consideran múltiples embalses en cascada y el efecto que la variación de la altura del salto tiene sobre la eficiencia de la operación. El efecto de la variación de la altura del salto, siendo no lineal, junto con la configuración hidráulica en cascada, vuelve el problema más complejo y de gran dimensión. Para su resolución, se considera un método de optimización basado en programación no lineal, siendo comparado con el método corrientemente utilizado, basado en la programación lineal. Los resultados de la simulación computacional demuestran que la programación no lineal es el método de optimización más adecuado.

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THEORY AND EXPERIMENT IN TEACHING ROBOTIC SYSTEMS AT ELECTRICAL ENGINEERING STUDENTS

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Publicado em:
17th EAEEIE Conference, Craiova, June 2006

This paper focuses on our method to provide the expertise that our students should acquire in Robotics as part of an Electrical Engineering degree.
Up to now Robotics has been an optional subject for these students. Both the theoretical component and the investment in training material were devoted to attract more students to the course as well as to achieve a number of learning objectives specified according to their background, industry needs and the scheduled course time.

CURRENT CONTROL OF A VENTURINI BASED MATRIX CONVERTER

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This paper defines the guidelines of a set of lectures for M.Sc. or Ph.D. students in electrical engineering. Often, these students are acquainted with the analysis and design of controllers for most power converters and electrical machines, using the Concordia and Park transformation. Based on these acquired skills, the main aim of this paper is to use a similar approach to define the main guidelines to design current controllers for matrix converters, using equivalent matrix converter dq models and considering two loads: resistiveinductive type and induction machines.

The matrix converter models have been obtained in previous works assuming ideal input and output filters, and are based on the inferring of Venturini modulation indexes in dq coordinates. Their main advantage is the decoupling of the output voltages and input currents, allowing the establishement of adequate and independent control actions for the output and input variables.

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Actas do International Symposium on Industrial Electronics, Montréal, Canadá, de 9 a 13 de Julho de 2006.

THOR: A TOOL FOR SCHOOL TIMETABLING

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Publicado em:
PATAT 2006, Practice and Theory of Automated Timetabling, pp 532-535, Agosto 2006

This system is the result of our previous work on the subject of school timetabling. It was designed to respond mainly to Portuguese schools from various educational levels. It consists of three main blocks; a graphical user interface; an automatic scheduler and a relational database. This system is now in use by more than 100 schools in Portugal with significant success (http://www.fmaismais.pt).

ANALYSIS OF THE SHORT-TERM PROFIT-BASED BEHAVIOR OF A HYDROELECTRIC ENERGY SYSTEM USING A NONLINEAR PROGRAMMING METHOD

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The electric energy market restructuring process has introduced power generation concurrency as well as the possibility of the consumer to choose which deliverer he or she wants. This new scenario brings new problems in electric energy management. One of these new problems is the short-term hydro scheduling (STHS) problem.
The STHS problem is treated as a deterministic one. Where the problem includes stochastic quantities, the corresponding forecasts are used. The hydroelectric generation characteristics are mainly assumed as linear or piecewise linear in hydro scheduling models, neglecting head variations. In hydroelectric power plants with a small storage capacity available, also known as run-of-the-river hydroelectric power plants, the power generation efficiency can change significantly due to the head change effect. Hence, it is necessary to consider the head change effect on STHS in order to obtain results that are more realistic. This paper presents a nonlinear programming method that considers not only that hydroelectric power generation is a function of the water discharge and of the head, but also that the maximum water discharge is head-dependent. The proposed method expresses hydro generation characteristics more accurately, providing a higher profit for the generating company with added advantage on acceptable computation time.

Publicado em:
Book of Proceedings of the 19th Mini-EURO Conference: Operation Research Models and Methods in the Energy Sector — ORMMES 2006, Coimbra, Portugal, 6-8 September, 2006, ISBN 989-95055-0-1.

APPLICATION OF NEURAL NETWORKS ON NEW-DAY ELECTRICITY PRICES FORECASTING

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Publicado em:
Book of Proceedings of the 41st International Universities Power Engineering Conference — UPEC 2006, Newcastle upon Tyne, UK, pp. 362-363 and CD-R, 6-8 September, 2006, ISBN 1-904794-19-X.

Next-day electricity price forecast has become a very helpful tool to consumers and to producers in managing their price risk and in planning the operations of their electric energy resources. Hence, in order to achieve better profits next-day electricity price forecast has become essential for developing bidding strategies and for developing information systems for bilateral contracts, that is, electricity price forecasting has become essential for developing negotiation skills in order to achieve better profits. There are several techniques, reported in the literature, to predict electricity prices. Reported techniques include traditional time series models, auto regressive - AR - models and auto regressive integrated moving average - ARIMA - models.
This paper presents an application for next-day electricity prices forecasting based on neural networks. Good forecasting tools hedging against daily price volatility are becoming increasingly important in nowadays competitive electricity markets, avowing misjudgement of future price movements and preventing considerable losses for consumers and producers. Next-day electricity price forecast is essential to consumers and to producers in planning the operations of their electric energy resources and for developing negotiation skills in order to achieve better profits. We evaluate the accuracy of the proposed application of neural networks for next-day electricity prices forecasting based on case studies for a real world electricity market and report our experience with this application.

OVERVIEW OF ECONOMIC AND ENVIRONMENTAL POLICY ISSUES AFFECTING THERMAL POWER SYSTEMS OPERATIONAL PLANNING UNDER DEREGULATION

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One of the major issues of introducing a system of emissions trading concerns the allocation of emission allowances to the participants of such a system. Emission allowances, which are given in tonnes of CO_2, entitle the holder to emit a corresponding amount of CO_2 during a specified period.

The environmental issues imposed by the Protocol of Kyoto imply new constraints in the operational planning of the thermal resources. Hence, thermal power systems operational planning should ensure both competitiveness to generating companies in the energy market and environmental protection by reducing emissions of greenhouse gases and other pollutants as an outcome of less consumption of fossil fuels.

This paper provides a review and general backgrounds of research and developments in the field of thermal power systems operational planning, namely on economic and environmental policy issues. On the one hand, within the energy market, operational planning has evolved from a minimum-cost policy in state-owned monopolistic companies to a profit-based policy under market conditions. On the other hand, as a consequence of growing environmental concern, an unprecedented change points to a scenario where it is necessary to take into account the constraints related to the environment. Consequently, operational planning of thermal power systems needs to be not only considered within the energy market, but also within preserving healthy conditions and self recovery cycles in the environment.

Publicado em:
Book of Proceedings of 41st Inter. Universities Power Engineering Conference — UPEC 2006, Newcastle upon Tyne, UK, 6-8 September, 2006, ISBN 1-904794-19-X.

BUS PLATFORM DESIGN FOR INTEGRATED FUEL CELL ELECTRIC VEHICLE

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Publicado em:
22nd International Batery, Hybrid and Fuel Cell Electric Vehicle Symposium & Exposition, (EVS22). Yokohama, Japan, 23-28 October 2006

In this paper the development of a new transportation platform is proposed, considering the specific power drive elements and focusing on the fuel cell accommodation. Massive changes are proposed at several layers of the resulting EV bus. This proposed transportation platform presents the following characteristics: low level ground floor, handicapped supporting structures, an open space body of the vehicle, non motorized spheres to support the weight of the vehicle, two independent traction units that allow simultaneously establishing the vehicle direction and hydrogen storage units placed on the vehicle roof.

ENERGY AND ENVIRONMENTAL IMPACTS OF PLUG-IN HYBRID ELECTRIC VEHICLES IMPLEMENTATION IN A TRANSPORTATION FLEET: APPLICATION TO A PORTUGUESE POSTAL SERVICES COMPANY

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The need of reducing greenhouse gases emissions (GGE), imposed by Kyoto protocol, has been an incentive to the implementation of environmental good-practices in several countries. Portugal is not an exception. However, the need for economic development and an higher quality of life induced more energy consumption and increasing the GGE.

Transportation economic sector will be, at 2010, the most important GGE responsible in Portugal, representing 29.0% of all CO_2 emissions. The main fraction of those emissions, 84.6%, corresponds to road transport activity.

Paper demonstrates that the implementation of alternative vehicle drivetrains, like HEV and PHEV, in the Portuguese automobile fleet could be a credible solution to the needed GGE reduction and can also contribute for attenuating the imported energy dependency of Portugal. That implementation could begin in transportation fleets that must hold the responsibility for their pollutant gaseous emissions.

The case study presented is applied to a Portuguese postal services company fleet showing the possibility of reducing in more than a half, at 2010, GGE and primary energy consumption, at the small vans segment, substituting conventional Diesel vehicles by PHEVs. Other PHEV advantage is the possibility to reduce urban noise and to avoid local pollutant gaseous emissions.

Publicado em:
The 22nd International Battery, Hybrid and Fuel Cell Electric Vehicle Symposium and Exposition, Yokohama, October 2006

REACTIVE POWER COMPENSATION USING SLIDING-MODE CONTROLLED THREE-PHASE MULTILEVEL CONVERTERS

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Publicado em:
12th Internacional Conference on Harmonics and Quality of Power. Cascais, Portugal 1-5 October 2006

This paper presents sliding-mode controlled multilevel converters for reactive power compensation. The reactive power compensation scheme here proposed includes a prototype three-phase multilevel converter and a digital signal processing system, in which sliding-mode and linear controllers are implemented. The instantaneous power theory is presented and used for reactive power compensation, together with the converter models needed for the application of the multilevel sliding-mode controllers and dc voltage capacitor equalization. Simulation and experimental results are shown in order to highlight the system operation and control robustness.

6DOF STEWART PLATFORM EMULATION OF A SELF-BALANCING TWO WHEELERS EV

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This work emulates on a 6DOF Stewart Platform the dynamic model of a self-balancing dual electric servo, stand-up device with two wheels that maintains vertical balance while moving forward and backwards, depending on the user body position. Also rotational displacements are incorporated in the device model.
The device dynamics, based on the dynamics of an inverted pendulum is a complex non-linear system. The inverted pendulum model used is based on an upright balanced rod with one angle deflection, mounted on a movable cart.
The device is powered by two Brushless DC motors controlled using hysteretic vectorial control.
Validation will be obtained by comparing the dynamic behaviour of the device and its implementation on the 6DOF Stewart Platform.

Publicado em:
Proceedings of the 22nd International Battery, Hybrid and Fuel Cell Electric Vehicle Symposium & Exposition (EVS22), p 1593-1603, (in CD-ROM). Yokohama, Japan, OCT. 26, 2006

SHORT-TERM SCHEDULING OF HEAD-DEPENDENT HYDRO POWER SYSTEMS: A QUADRATIC OPTIMIZATION APPROACH

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Publicado em:
Journal WSEAS Transactions on Systems, November 2006, Vol. 5, No. 11, ISSN 1109-2777, pp 99-224.

This paper combines management knowledge of head-sensitive hydro plants with computer simulation methods based on linear and non-linear network programming, on the assessment of accurate short-term decisions for the hydroelectric energy, article of trade, under profit-based environment. Under profit-based environment, the optimal scheduling of the hydroelectric facilities available is essential for generating companies to face competitiveness. Moreover, also responds to climate change contributing to reduce fossil fuels energy dependency. In a competitive energy market, generation companies have to maximize their profits selecting the best strategy. The schedule is formulated as an optimal trade-off problem of how to make the present profit by the management of the water available for power generation without compromising future potential profit. Comparison between traditional linear network programming scheduling that ignores head dependency, with the non-linear one, reveals that reservoirs should operate at an appropriated storage level to benefit power generation efficiency, giving a higher global profit for the generation company with negligible extra CPU-time required.

ENERGIAS RENOVÁVEIS NO DESEQUILÍBRIO ENTRE A PRODUÇÃO E O CONSUMO: PERSPECTIVAS PARA PORTUGAL NO PERÍODO 2010 – 2025

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O compromisso assumido com a assinatura do protocolo de Quioto e a necessidade de redução das implicações ambientais e da dependência externa associadas ao crescente consumo de energia em Portugal, têm sido motivo para um ambicioso plano de desenvolvimento e instalação de fontes de energia renováveis.
Ao longo do período 2006-2025, espera-se um importante investimento na capacidade de produção de energia eléctrica a partir de fontes renováveis. Prevê-se que já no ano 2010, 45% da energia eléctrica consumida em Portugal tenha origem renovável.
A crescente integração de fontes renováveis no sistema electroprodutor português, para além dos indiscutíveis benefícios já apresentados e devidamente discutidos nos mais variados fóruns, poderá também introduzir algumas questões especialmente relacionadas com o planeamento e operação do sistema eléctrico.
A imprevisibilidade da disponibilidade de produção das fontes renováveis associada às variações temporais da procura de energia pode resultar em desequilíbrios entre produção e consumo, que devem estar devidamente estudados, previstos e quantificados, de modo a que possam ser colmatados o mais eficazmente possível.

Publicado em:
Actas do IST Fórum Energia – Outono 06, Lisboa, Portugal, Novembro de 2006.

APROVEITAMENTOS HIDROELÉCTRICOS COM QUEDA DEPENDENTE: NOVA METODOLOGIA PARA A OPTIMIZAÇÃO DA EXPLORAÇÃO

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Publicado em:
Actas do IST Forum Energia — Outono 06, Lisboa, Portugal, 16 de Novembro, 2006.

Os aproveitamentos hidroeléctricos contribuem para a contenção das emissões de gases com efeito de estufa, o que constitui uma vantagem ambiental face às centrais térmicas. Ainda, estes aproveitamentos apresentam uma grande flexibilidade na sua operação, quando explorados convenientemente. Sob o ponto de vista energético existe uma característica discernível típica dos aproveitamentos hidroeléctricos, derivada da capacidade potencial da afluência hídrica ter a sua valorização em termos energéticos dependente da diferença de potencial útil do campo de gravidade e não só em massa como no caso das centrais térmicas, visto que, um mesmo volume significa potencialidades de produção diferentes consoante a altura de queda que caracteriza o recurso — efeito de queda. Cada aproveitamento hidroeléctrico é caracterizado por uma relação de três variáveis: potência, caudal turbinado e altura de queda. Essa relação é não linear e não convexa. O efeito de queda, tipicamente desprezado ou simplificado em metodologias baseadas em optimização linear, é especialmente relevante nos aproveitamentos a fio de água. Essa é a situação por exemplo no Douro. Uma dificuldade acrescida resulta da dependência não linear da altura de queda em relação ao caudal turbinado, sendo que quanto maior for o caudal turbinado menor será a altura de queda devido à elevação da cota de jusante e diminuição da cota de montante. Esta comunicação propõe uma nova metodologia baseada em optimização não linear para a exploração de aproveitamentos hidroeléctricos com queda dependente, sendo apresentados e discutidos os resultados obtidos.

DIGITAL IMPLEMENTATION OF A DC BUS VOLTAGE CONTROLLER FOR FOUR-WIRE ACTIVE FILTERS

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Voltage regulation systems play an important role in all self-powered systems connected to the ac mains, like active filters (AF's), unified power flow controllers (UPFC's), advanced static VAr compensators (ASVC's), PWM rectifiers, uninterruptible power supplies (UPS's) and neutral current compensators (NCC's). In some of these applications the voltage regulation is not the primary goal. However, voltage regulation is absolutely necessary to the operation of the voltage source converters (VSC's) in order to sink or feed current into mains. When neutral current control is desirable, especially in active filtering with zero sequence current component compensation, three-phase four-wire converters are needed. They can be realized either with a three-leg VSC with split dc link capacitor, as in the present study, or with a four-leg VSC. When dealing with neutral current a special care should be taken into account in order to assure an equal voltage sharing between capacitors. Also, the ripple voltage must be considered so that the rated capacitor voltages are not exceeded. These problems are due to neutral current caused by unbalance or current harmonics.

Some works have been realized in the design of voltage controllers for these converters using linear and sliding-mode control techniques. The works realized are based on linear models and analog control, however digital implementation issues need to be presented and discussed. In this paper a digital control system that performs the voltage regulation on an AF, based upon a three-leg VSC with split dc link capacitor is presented. Experimental results in a DSP platform are presented to highlight the system characteristics with respect to dynamic and steady-state behaviour.

Publicado em:
IEEE-IECON'06 "32nd Annual Conference of the IEEE Industrial Electronics Society", Paris - França, Novembro, 2006.

INDUSTRIAL FIELDBUS TECHNOLOGY FROM A TEACHING POINT OF VIEW

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Publicado em:
International Journal of Computer Applications in Technology, Vol. 25, No. 4, 2006

ABSTRACT

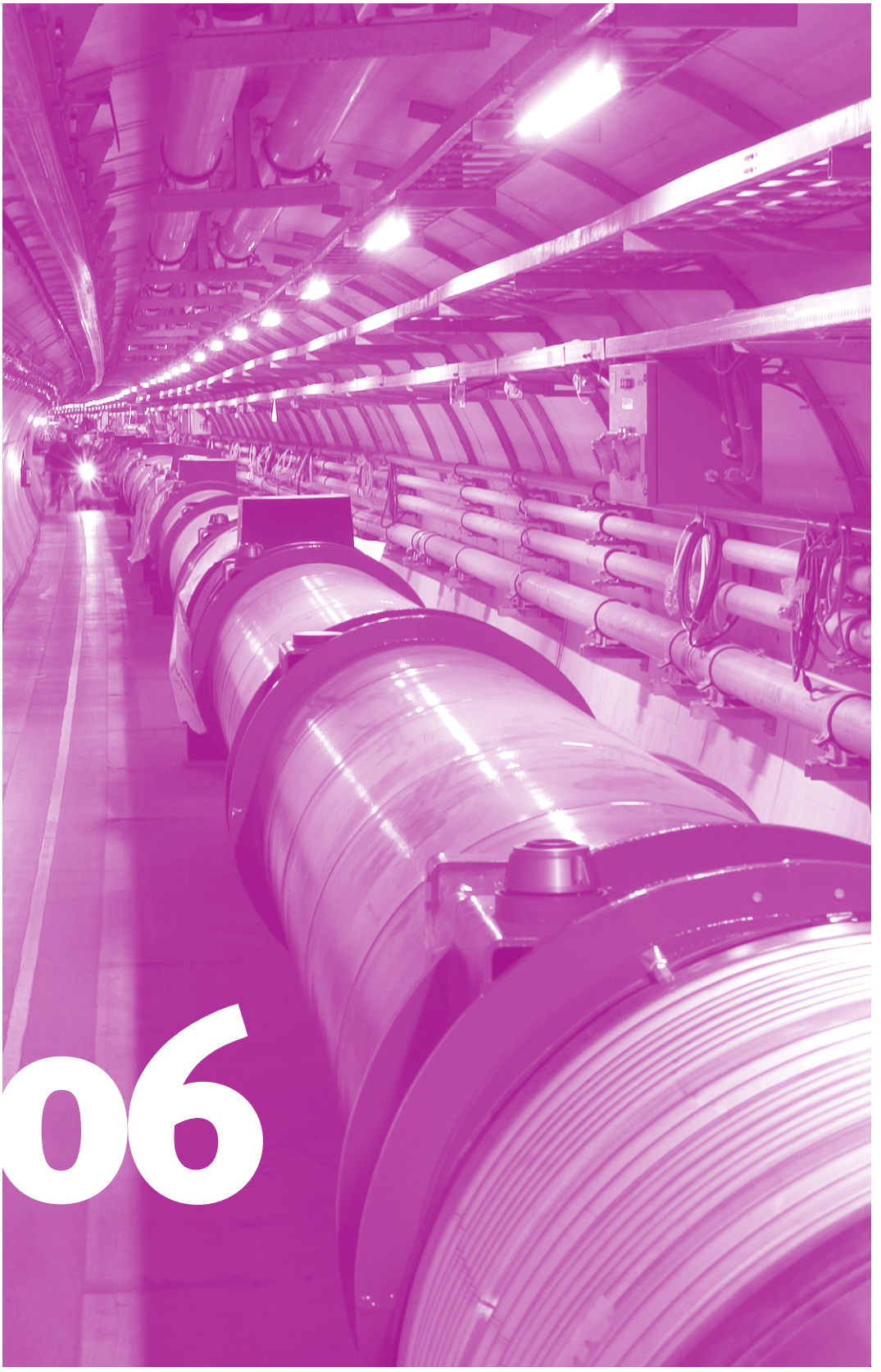
This paper presents a discussion on fieldbus technologies as a part of the required competencies in modern electrical engineering graduations. Fieldbus systems are fast changing technologies of great importance for electrical and automation engineers deserving a special investment of university curricula and laboratory resources owing to their essential role in modern industrial automation and control practice. Their diversity as well as their permanent and fast evolution is a challenge for teaching, both in terms of curriculum design and logistic support. Historical facts and actual tendencies are at the starting point of our analysis, leading to the proposed methodological approach to the theoretical and experimental teaching components.

PREVISÃO DE POTÊNCIA EM GERADORES EÓLICOS

Fonte, Pedro Miguel Neves

Mestrado em: Engenharia Electrotécnica e Computadores
Grau concedido por: Instituto Superior Técnico
Orientador: Rui Manuel Gameiro de Castro
Co-orientador: José Carlos Lourenço Quadrado
Provas concluídas em: 24 de Maio de 2006

Portugal pretende aumentar a capacidade da energia produzida através de recursos renováveis, de modo a reduzir a dependência dos combustíveis fósseis, objectivando atingir em 2010, 3750 MW de potência instalada em aerogeradores. Esta potência instalada poderá provocar problemas no sistema electroprodutor, uma vez que a produção de energia eléctrica em parques eólicos segue as variações da velocidade do vento, tornando-se assim importante conseguir previsões fiáveis para vários horizontes temporais.
Neste trabalho, estuda-se a capacidade de previsão da velocidade do vento e consequentemente da potência disponível, com o horizonte de uma hora, através de redes neuronais artificiais do tipo Perceptrão Multicamada, usando como algoritmo de aprendizagem a retropropagação dos erros.
Abordam-se igualmente as variáveis mais importantes na produção de energia em aerogeradores, bem como os fenómenos que as influenciam. Escolhem-se as grandezas do conjunto de dados para a previsão da velocidade do vento, elaborando-se conjuntos de padrões para a aprendizagem da rede neuronal e definem-se estratégias para a aprendizagem a nível da arquitectura e número de iterações.
Fazem-se ensaios com redes com diversas arquitecturas e diversos conjuntos de dados, escolhendo-se a que apresenta a melhor generalização. Validam-se os resultados comparando-os com métodos de previsão a curto prazo considerados como de referência.



06

FÍSICA

Anuário Científico 2006

ISEL

CVD OF CrO_2: TOWARDS A LOWER TEMPERATURE DEPOSITION PROCESS

Sousa, P.M.[1]; Dias, S.A.[1]; Silvestre, A.J.[2]; Conde, O.[1]; Morris, B.[3]; Yates, K.A.[3]; Branford, W.R.[3,4]; Cohen, L.F.[3]

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We report on the synthesis of highly oriented a-axis CrO_2 films onto (0001) sapphire by atmospheric pressure CVD from CrO_3 precursor, at growth temperatures down to 330 degree Celsius, i.e. close to 70 degrees lower than in published data for the same chemical system. The films keep the high quality magnetic behaviour as those deposited at higher temperature, which can be looked as a promising result in view of their use with thermally sensitive materials, e.g. narrow band gap semiconductors.

Publicado em:
Chemical Vapor Deposition, 12 (2006) 712.

CVD OF CrO_2 THIN FILMS: INFLUENCE OF THE DEPOSITION PARAMETERS ON THEIR STRUCTURAL AND MAGNETIC PROPERTIES

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Publicado em:
Material Science Forum, 514 (2006) 289.

This work reports on the synthesis of CrO_2 thin films by atmospheric pressure CVD using chromium trioxide (CrO_3) and oxygen. Highly oriented (100) CrO_2 films containing highly oriented (0001) $Cr2O_3$ were grown onto Al_2O_3 (0001) substrates. Films display a sharp magnetic transition at 375 K and a saturation magnetization of 1.92 μ_B/f.u., close to the bulk value of 2 μ_B/f.u. for the CrO_2.

OPTIMISATION OF RODRUN LC300/PP COMPATIBILISED BLENDS: INFLUENCE OF THE COMPATIBILISER AND LCP CONTENTS ON THE RHEOLOGICAL, MORPHOLOGICAL AND MECHANICAL PROPERTIES

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The present study focuses on the optimisation of LCP/TP compatibilised systems. This study was essentially devoted to the influence of different LCP and compatibiliser contents on the final morphological, rheological and mechanical properties of the blends. Rheologically, we used both standard small amplitude oscillatory shear and large amplitude oscillatory shear (LAOS) experiments in order to improve the understanding of the mechanisms behind the mechanical reinforcement that might be helpful in the optimisation of liquid crystalline polymer and thermoplastic blends. The results revealed that LAOS, in particular, is highly sensitive to different morphologies and may be correlated with the effectiveness of compatibilisers, which is not surprising since the flow behaviour of LCPs is highly complex and non-linear, with lower non-linear characters obtained for those blends that showed a higher fibrillar formation and better mechanical properties.

Publicado em:
Journal of Polymer Engineering, 26 (2006) 511.

DIFFUSION-LIMITED DEPOSITION WITH DIPOLAR INTERACTIONS: FRACTAL DIMENSION AND MULTIFRACTAL STRUCTURE

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Publicado em:
Journal of Chemical Physics, 124 (2006) 064706.

Computer simulations are used to generate two-dimensional diffusion-limited deposits of dipoles. The structure of these deposits is analyzed by measuring some global quantities: the density of the deposit and the lateral correlation function at a given height, the mean height of the upper surface for a given number of deposited particles, and the interfacial width at a given height. Evidences are given that the fractal dimension of the deposits remains constant as the deposition proceeds, independently of the dipolar strength. These same deposits are used to obtain the growth probability measure through the Monte Carlo techniques. It is found that the distribution of growth probabilities obeys multifractal scaling, i.e., it can be analyzed in terms of its $f(\alpha)$ multifractal spectrum. For low dipolar strengths, the $f(\alpha)$ spectrum is similar to that of diffusion-limited aggregation. Our results suggest that for increasing the dipolar strength both the minimal local growth exponent α_{min} and the information dimension D_1 decrease, while the fractal dimension remains the same.

PHASE TRANSITION IN TWO-DIMENSIONAL DIPOLAR FLUIDS AT LOW DENSITIES

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Monte Carlo computer simulations of a quasi two-dimensional (2D) 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 (or mass) distributions is used to obtain approximations to their partition functions. Within the scope of these approximations, the results of this work suggest that the 2D dipolar fluid 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:
Physical Review E, 73 (2006) 041507.

STABILITY OF THE NORMAL VACUUM IN MULTI-HIGGS-DOUBLET MODELS

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We show that the vacuum structure of a generic multi-Higgs-doublet model shares several important features with the vacuum structure of the two and three Higgs-doublet model. In particular, one can still define the usual charge breaking, spontaneous CP breaking and normal (charge and CP preserving) stationary points. We analyse the possibility of charge or spontaneous CP breaking, by studying the relative depth of the potential in each of the possible stationary points.

Publicado em:
Physical Review D, 74 (2006) 085016.

06

LOOKING FOR DELTA I = 5/2 AMPLITUDE COMPONENTS IN B ---› PI PI AND B ---› RHO RHO EXPERIMENTS

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We discuss how experiments measuring B ---› pi pi and B ---› rho rho may be used to search for a Delta I = 5/2 amplitude component. This component could be the explanation for a recent (albeit very tentative) hint from B(Bbar) ---› rho rho decays that the isospin triangles do not close.

Publicado em:
Physical Review D, 73 (2006) 071501.

TUNEABLE MICRO- AND NANO-PERIODIC STRUCTURES IN A FREE-STANDING FLEXIBLE URETHANE/UREA ELASTOMER FILM

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Publicado em:
European Physical Journal E, 21 (2006) 319.

We have studied the control and manipulation of tuneable equilibrium structures in a free-standing urethane/urea elastomer film by means of atomic force microscopy, small-angle light scattering and polarising optical microscopy. The urethane/urea elastomer was prepared by reacting a poly(propyleneoxide)-based triisocyanate-terminated pre-polymer (PU) with poly(butadienediol) (PBDO), with a weight ratio of 60%PU/40%PBDO. An elastomer film was shear-cast onto a glass plate and allowed to cure, first in an oven, then in air. Latent micro- and nano-periodic patterns are induced by ultra-violet (UV) irradiation of the film and can be "developed" by applying a plane uniaxial stress or by immersing the elastomer in an appropriate solvent and then drying it. For this elastomer we describe six pattern states, how they are related and how they can be manipulated. The morphological features of the UV-exposed film surface can be tuned, reproducibly and reversibly, by switching the direction of the applied mechanical field. Elastomers extracted in toluene exhibit different surface patterns depending upon the state in which they were developed. Stress-strain data collected for the films before and after UV irradiation reveal anisotropy induced by the shear-casting conditions and enhanced by the mechanical field. We have interpreted our results by assuming the film to consist of a thin, stiff surface layer ("skin") lying atop a thicker, softer substrate ("bulk"). The skin's higher stiffness is hypothesised to be due to the more extensive cross-linking of chains located near the surface by the UV radiation. Patterns would thus arise as a competition between the effects of bending the skin and stretching/compressing the bulk, as in the work of Cerda and Mahadevan [Phys. Rev. Lett. **90**, 074302 (2003)]. We present some preliminary results of a simulation of this model using the Finite Element package ABAQUS.

SIMPLE MODEL FOR BIAXIAL SMECTIC-A LIQUID CRYSTAL PHASES

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We have generalised the McMillan theory of liquid crystalline smectic order in uniaxial particle fluids to biaxial particles. Upon varying the control parameter, a uniaxial nematic phase may: (i) order biaxially first, then smectically; (ii) order smectically first, then biaxially; (iii) simultaneously order biaxially and smectically. We investigate, in the limit of complete orientational order of the molecular major axes, which of these scenarios are realised for a simple model of particles with the symmetry of rectangular parallelepipeds. We also present a generic variational derivation of the theory based on the identification of the dominant order parameters for the most ordered phase.

Publicado em:
Physical Review E, 73 (2006) 061708.

ELLIPTICAL SOFT COLLOIDS IN SMECTIC-C FILMS

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Publicado em:
Physical Review E, 74 (2006) 021706.

We investigate theoretically the elliptical shapes of soft colloids in freely standing smectic-C films, that have been reported recently. The colloids favor parallel alignment of the liquid crystal molecules at their surfaces and, for sufficiently strong anchoring, will generate a pair of defects at the poles of the colloidal particles. The elastic free energy of the liquid crystal matrix will, in turn, affect the shape of the colloids. In this study we will focus on elliptical soft colloids and determine how their equilibrium shapes depend on the elastic constants of the liquid crystal, the anchoring strength, the surface tension, and the size of the colloids. A shape diagram is obtained analytically, by minimizing the Frank elastic free energy, in the limit of small eccentricities. The analytical results are verified, and generalized to arbitrary eccentricities, by numerical minimization of an appropriate Landau free energy. The latter is required for an adequate description of the topological defects when the liquid crystal correlation length is comparable to the size of the colloidal particles.

AZORES HOTSPOT SIGNATURE IN THE UPPER MANTLE

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The Azores archipelago occupies a lateral branch of the Mid-Atlantic Ridge near the triple junction of three large tectonic plates, the North American, the Eurasian and the African plates. The tectonic setting is even more complex because of the existence of the Azores hotspot and hotspot–ridge interaction. However, the hotspot origin at depth as a plume and its lateral extent are controversial subjects. High-resolution tomographic models, through the mapping of low-velocity and anisotropy anomalies, can provide an important hint to evaluate the depth and lateral extent of plumes when they exist. Therefore, we present a review of the Azores deep seismic structure as inferred from recent global and regional studies. The mapping of S-wave negative velocity anomalies in various models reveals a negative anomaly beneath the Azores confined within the upper 250–300 km. Considering the time evolution of a plume, this low-velocity anomaly might be the signature of a present-day dying plume, which created the Azores plateau 20 Ma ago. However, tomographic investigations have reached the limit of resolution provided by the global and regional seismic coverage available today. Only a long-term deployment (several years) of several broadband seismic stations in the Archipelago and on the surrounding seafloor will provide the increased resolution to better characterize plume geometry.

Publicado em:
Journal of Volcanology and Geothermal Research, 156 (2006) 23.

AS FORÇAS DA NATUREZA: A IMPORTÂNCIA, BELEZA E SIMPLICIDADE DE FORÇA ELECTROMAGNÉTICA

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Publicado em:
Gazeta de Física, 29 (3) (2006) 28.

A Física é a Ciência que estuda os fenómenos naturais em todas as escalas. Apesar da infinidade de fenómenos, estão-lhe subjacentes apenas quatro forças: a gravítica, a electromagnética, a fraca, e a forte. A força electromagnética é a mais relevante para a compreensão da esmagadora maioria dos fenómenos do nosso dia-a-dia. Numa síntese de grande beleza, Maxwell mostrou que o electromagnetismo se resume a quatro "frases", que muito impressionaram Einstein.

SPIN TRANSPORT PROPERTIES OF HIGHLY-ORIENTED CrO_2 FILMS ON AL_2O_3 (0001)

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We report on the synthesis of and electronic characterization of CrO_2 thin films, grown on Al_2O_3(0001) by atmospheric pressure CVD. The highly-oriented (100) CrO_2 films also contain a highly-oriented (0001) Cr_2O_3 phase. The films display a sharp magnetic transition at 375 K and a saturation magnetization of 1.92 μ_B/f.u., close to the bulk value of 2 μ_B/f.u. for CrO_2. The spin polarization and spin transport is studied both in the film bulk and at the surface with complementary point-contact Andreev reflection, resistivity and Hall transport measurements. The effect of surface degradation on the transport properties is discussed with reference to applications.

Publicado em:
Livro de resumos da conferência "Condensed Matter and Materials Physics Conference", CMMP 2006, Institute of Physics, University of Exeter, UK (comunicação em poster).

THE EFFECT OF DISORDER ON THE RESISTIVITY AND ANOMALOUS HALL EFFECT IN CrO_2 THIN FILMS

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Publicado em:
Livro de resumos da conferência "Current Research in Magnetism", CRIM'06, Imperial College, London, UK, 2006 (comunicação em poster).

CrO_2 has attracted a great deal of interest because it has been shown to have a very high degree of spin polarization of the transport current. In CrO_2 samples with low disorder, although the residual resistivity is very low, the resistivity is very strongly temperature dependent above 100K, and only below 100K does it have the resistivity expected of a "good metal". It is interesting that the anomalous Hall effect, which has been associated with both scattering and intrinsic (loss-free) processes, vanishes below 100K. Here we compare the temperature dependence of the resistivity, and of the anomalous Hall resistivity, of a series of CrO_2 films grown at different deposition temperatures by chemical vapour deposition on sapphire substrates. As the deposition temperature decreases the residual resistivity of the films increases by an order of magnitude, indicating a strong increase in disorder in the films. The role of this disorder in the anomalous Hall effect in CrO_2 is discussed.

STRUCTURE AND SPIN TRANSPORT PROPERTIES OF CrO_2 FILMS GROWN BY CVD AT MODERATE TEMPERATURE

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Chromium dioxide (CrO_2) is one of the most attractive ferromagnetic compounds being investigated for potential use in spintronic devices. Many of the proposed devices demand carefully controlled growth of interfaces that can be achieved by preparing thin films at sufficiently low temperatures to ensure interface quality and avoid substrate damage. Up to now, the most successful technique reported in literature for the deposition of high quality ferromagnetic CrO_2 thin films is based on the thermal decomposition of CrO_3 on oriented TiO_2 and Al_2O_3 substrates at temperatures of ~390ºC.

In this work, we report on improvements made towards the growth of CrO_2 thin films at lower temperature by atmospheric pressure CVD. X-ray diffraction results demonstrate the synthesis of highly oriented a-axis CrO_2 films by thermal decomposition of CrO_3 onto Al_2O_3 (0001) substrates heated at temperatures as low as 330 ºC. The study of the CrO_2 growth rates as a function of the deposition temperature allowed to evaluate the apparent activation energy and to assess the deposition mechanism.

The spin polarization and spin transport was studied both in the film bulk and at the surface with complementary point-contact Andreev reflection, resistivity and Hall transport measurements. Andreev reflection measurements indicate that spin transport polarisation is of the order of 70-80% at 4.2K.

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Livro de resumos da conferência "Junior EUROMAT 2006", Lusanne, Switzerland, 2006 (comunicação em poster).

TUNEABLE MICRO- AND NANO-PERIODIC STRUCTURES IN A FREE-STANDING FLEXIBLE URETHANE/UREA ELASTOMER FILM

Godinho, M.H.[1]; Trindade, A.C.[1]; Figueirinhas, J.L.[2,3]; Melo, L.V.[3]; Brogueira, P.[3,4]; Deus, A.M.[4,5]; Teixeira, P.I.C.[6]

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Publicado em:
Livro de resumos da conferência "International Workshop on Mesoscale and Multiscale Description of Complex Fluids", iwmcof2006, Monash University, Prato, Italy, 2006 (comunicação em poster).

We have studied the control and manipulation of tuneable equilibrium structures in a free-standing urethane/urea elastomer film by means of atomic force microscopy, small-angle light scattering and polarising optical microscopy. The urethane/urea elastomer was prepared by reacting a poly (propyleneoxide)-based triisocyanate-terminated prepolymer (PU) with poly (butadienediol) (PBDO), with a weight ratio of 60%PU/40%PBDO. An elastomer film was shear-cast onto a glass plate and allowed to cure, first in an oven, then in air. Latent micro- and nano-periodic patterns are induced by ultra-violet (UV) irradiation of the film and can be "developed" by applying a plane uniaxial stress or by immersing the elastomer in an appropriate solvent and then drying it. For this elastomer we describe six pattern states, how they are related and how they can be manipulated. The morphological features of the UV-exposed film surface can be tuned, reproducibly and reversibly, by switching the direction of the applied mechanical field. Elastomers extracted in toluene exhibit different surface patterns depending upon the state in which they were developed. Stress-strain data collected for the films before and after UV irradiation reveal anisotropy induced by the shear-casting conditions and enhanced by the mechanical field. We have interpreted our results by assuming the film to consist of a thin, stiff surface layer ("skin") lying atop a thicker, softer substrate ("bulk"). The skin's higher stiffness is hypothesised to be due to the more extensive cross-linking of chains located near the surface by the UV radiation. Patterns would thus arise as a competition between the effects of bending the skin and stretching/compressing the bulk, as in the work of Cerda and Mahadevan [Phys. Rev. Lett. 90, 074302 (2003)]. We present some preliminary results of a simulation of this model using the Finite Element package ABAQUS.

ENERGY AND TENSION OF FILMS AND PLATEAU BORDERS IN A FOAM

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We discuss a number of problems relating to the energy and geometry of liquid foams in three dimensions. We use Plateau's concept of a skeletonised or ideal dry foam, consisting of geometrical surfaces, lines and points, which correspond, respectively, to the films, Plateau borders and nodes of the real foam, but including the contributions of all these elements to the total foam energy (and not just the film energy, as is usually done). In order to be able to write down all these contributions for a real foam, we conjecture that the same can be skeletonised by successively replacing the films by their mid-surfaces, the Plateau borders by the edges along which the mid-surfaces meet, and the nodes by the points where four edges are joined. We then relate the film energy γ and the film tension σ (energy per unit area), and define a Plateau border line tension τ (energy per unit length) and a node energy ν. The Plateau border line tension is negative and causes deviations from 120º of the angles between films, and from $\cos^{-1}(-1/3)$ of the angles between lines at nodes. We further define the excess energy ε of a Plateau border relative to the dry line. We illustrate our findings with calculations performed for a few simple systems — the double bubble, the lens bubble, and a bubble at a plate — for which skeletonisation is straightforward, and show that $\tau = \varepsilon/2$ when $\varepsilon \propto A^{1/2}$, with A the Plateau border cross-sectional area, i.e., for not too high liquid fractions.

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Livro de resumos da conferência "EUFOAM 2006", Potsdam, Germany, 2006 (comunicação oral).

INSTABILITIES IN TWO-DIMENSIONAL MULTI-LAYER BUBBLE CLUSTERS

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Publicado em:
Livro de resumos da conferência "EUFOAM 2006", Potsdam, Germany, 2006 (comunicação em poster).

We assess the stability of simple two-dimensional clusters of bubbles relative to small displacements of the vertices, at fixed bubble areas. The clusters analysed are: 1) flower clusters consisting of a central bubble of area λ surrounded by N shells each containing n bubbles of unit area, 2) periodic chain clusters consisting of N "parallel" rows of n bubbles of unit area and width w. The energy and bubble pressures of the symmetrical, unbuckled clusters are found analytically as a function of λ and w for given N and n. Both types of clusters studied show a single energy minimum at a critical λ_m or w_m. At the energy minimum for flower clusters, the pressure in the central bubble vanishes. The clusters show a symmetry-breaking buckling instability under compression at a critical λ_b or w_b. The corresponding critical energy E_b was determined with the Surface Evolver software. While for N=1 the conditions $\lambda_b = \lambda_m$, $w_b = w_m$ and $E_b = E_m$ hold, for N>1 buckling requires further compression beyond the minimum, for which the energy increases with increasing compression (decreasing λ or w), and the excess pressure in the central bubble of the flower clusters becomes negative.

$Y_3Os_8B_6$: A NEW BORIDE SUPERCONDUCTOR

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A new ternary boride, $Y_3Os_8B_6$, was prepared by arc melting. This compound crystallizes in a new structure type, which is closely related with the $CeCo_3B_2$-type. Ac-susceptibility, magnetization and resistivity measurements show that this compound is a new type II superconductor, with T_c = 5.5 K. The structure and properties of this compound are discussed in relation to other ternary superconducting borides.

Publicado em:
Livro de resumos da conferência "8th Prague Colloquium on f-Electron Systems", Prague, Czech Republic, 2006 (comunicação oral).

AFTERSHOCK SEQUENCE OF JULY 1998 FAIAL AND PICO ISLANDS (AZORES): AN ANALYSIS OF WAVEFORM SIMILARITIES, SEISMIC ANISOTROPY AND CRUSTAL STRUCTURE

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Publicado em:
Eos Trans. AGU, 87 (52), Fall Meet. Suppl., Abs. S53A-1311, 2006.

The Azores archipelago (Portugal) is located at an oceanic plateau, in a geodynamic environment prone to intense seismic and volcanic activity. On July 9th 1998, a 5.8 ML earthquake occurred near Faial Island, causing 10 casualties and severe destruction. The focal mechanism showed a strike-slip event with nodal planes striking N241E and N151E. This shock triggered a seismic swarm of thousands of events recorded by 14 stations located in the islands surrounding the epicentral area. Following a 1-D inversion with 735 selected events, we performed a waveform similarity analysis to enhance the hypocentral location and identify clusters of similar earthquakes. The clusters obtained, together with the composite focal mechanism solution, allowed the definition of the main active structures. The spatial distribution of events is more organized, concentrated in the middle-lower crust. The revision of the focal mechanisms of the best-constrained aftershocks showed that the swarm reactivated other faults besides the one associated with the main event. Single and composite solutions of focal mechanisms allowed inferring the maximum horizontal stress directions. An analysis of shear-wave splitting was performed, using the data generated by this seismicity, with the fast S-wave polarization direction showing to be stable for the majority of the seismic stations. Thus, it was possible to infer the direction of the maximum horizontal stress under the digital stations. These results showed to be coherent with the parameters obtained from the composite mechanisms solution, showing a rotation of SHmax from east to west.
To investigate the crustal structure in this volcanic region, we have conducted a local earthquake tomography study. The results are coherent with the presence of magmatic chambers beneath the main volcanic structures, and small-scale structures probably corresponding to solidified plugs or pockets of magma. A high Vp and low Vp/Vs oval body was found located at mid-lower crust and coincident with the orientation NNW-SSE of the most active seismogenic structure. This body may correspond to a plutonic intrusion that used a pre-existent deep fault to its emplacement. The crustal thickness under the islands volcanic buildings of Faial-Pico area was estimated on 14 km.

ELLIPTIC INCLUSIONS IN SMECTIC -C FILMS

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We present a theoretical investigation on the elliptical shapes of soft colloids in freely standing smectic C films, that have been reported in recent experiment [1]. The colloids favour parallel alignment of the liquid crystal molecules at their surfaces and, for sufficiently strong anchoring, will generate a pair of defects at the poles of the colloidal particles. In turn, the elastic free energy of the liquid crystal will affect the shape of the colloids. In this presentation we will focus on elliptical soft colloids and determine how their equilibrium shapes depend on the elastic constants of the liquid crystal, the anchoring strength, the surface tension and the size of the colloids.

A shape diagram is obtained analytically, by minimizing the Frank elastic free energy, in the limit of small eccentricities. The analytical results are verified, and generalized to arbitrary eccentricities, by numerical minimization of an appropriate Landau free energy. The latter is required for an adequate description of the topological defects when the liquid crystal correlation length is comparable to the size of the colloidal particles.

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Livro de resumos da conferência "Colloids, Interfaces and Liquid Crystals", Erice, Itália, 2006 (comunicação oral).

NEMATIC WETTING TRANSITION ON WEDGE-SHAPED SUBSTRATES

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We investigate the wetting behavior of a nematic at a wedge shaped substrate favoring homeotropic anchoring. The substrate induces a distortion of the nematic director, and an effective long-range interaction with the nematic-isotropic interface. We have used the Landaude Gennes energy to numerically obtain the wetting phase diagram, which now depends on the wedge angle.

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Livro de resumos da conferência "Colloids, Interfaces and Liquid Crystals", Erice, Itália, 2006 (comunicação em poster).

TWIST TRANSITION OF NEMATIC LIQUID CRYSTALS IN PATTERNED CELLS. EFFECT OF CONFINEMENT AND ELECTRIC FIELD

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We generalize the study of the geometrically-controlled twist in nematic cells [1] by taking into account the effect of the electric field. Standard minimization methods are not applicable to this problem since the functional hás no mínima in the presence of the electric field and constant potential boundary conditions. We perform artificial relaxation timestep using finite element methods together with adaptive meshes to compute direct solutions of the Euler-Lagrange equations satisfied by the extrema of the free energy functional.

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EFFECT OF SALT MARSH PLANTS IN THE MOBILITY OF CR IN SEDIMENTS

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Publicado em:
Livro de resumos do XIII Seminário Ibérico de Química Marinha, IPIMAR, Lisboa, Portugal, 2006 (Comunicação em poster e flash).

Plants growing in these soils or sediments are capable of extracting heavy metals and accumulating them in their tissue. Metal accumulation in plant parts and metal profiles in sediment may provide valuable information on the knowledge of the rhizosphere processes affecting the mobility of metals. Sediment cores with 50-cm depth were collected in nonvegetated area and in plots of *Halimione portulacoides* from two salt marshes (Rosário and Pancas) of the Tagus estuary. Layers of 1 to 5 cm thickness were sliced from each core and roots separated and cleaned from particles. Sediment and roots Samples were completely digested with a mixture of acids and determined total concentrations of Fe, Mn, Cr. The fractions of these metals extracted by hydroxylamine (HYD) and HCl were also quantified in sediment samples. Edaphic conditions of the sediment (O_2, pH, E_H, AVS and root biomass) were also characterized in both marshes. Higher dissolved oxygen concentration was found at depths with increased root biomass. Otherwise AVS was nearly absent in the root zone increasing at deeper layers. Total metal concentrations in sediments colonised by *H. portulacoides* showed higher variability with depth in comparison with non-vegetated sediments. Scattering may result from intense metal exchanges between plant belowground material and surrounding sediment. Higher concentrations of Fe_{HYD} (mainly Fe oxyhydroxides) were found in the rooting sediments as a result of oxidation of Fe(II) through the O_2 released by roots. The normalization of Cr_{HYD} levels in sediments to Fe_{HYD} showed a sharp increase when oxygen is depleted. This suggests that Cr is sequestered within the Fe oxyhydroxides fraction in the rooting zone with no oxygen. Surprisingly, roots of *H. portulacoides* from both marshes showed low ability to take up and accumulate Cr. A possible explanation is the reduction of soluble Cr(VI) to the stable Cr(III) and subsequent retention in the Fe oxyhydroxide fraction and not mobilised towards the roots. Thus, the inability or defense mechanisms of *H. portulacoides* to accumulate these Cr indicate that are ineffective for their phytostabilization.

ACÚSTICA AMBIENTAL. INFRA-ESTRUTURAS DE TRANSPORTE

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As infra-estruturas de transporte rodoviário, ferroviário e aéreo constituem uma importante fonte de ruído poluidora do ambiente sonoro. Por este facto, o projecto de novas estradas, linhas de caminho-de-ferro e aeroportos, bem como a alteração/beneficiação das existentes, deve tomar em linha de conta o ambiente acústico local e a previsão da sua alteração após a plena exploração de cada infra-estrutura de transporte.

Assim, o Estudo Acústico subsequente é indispensável e deve compreender as seguintes 4 fases distintas e complementares: i) Situação de Referência; ii) Impactes no Ambiente Sonoro; iii) Medidas Minimizadores de Ruído; iv) Programa de Monitorização de Ruído.

Estas 4 fases, quando elaboradas atempadamente e por técnicos qualificados, permitirão que a análise e a aprovação pelas Entidades Competentes das medidas de controlo de ruído preconizadas, seja eficaz e de modo a garantir que o desenvolvimento da rede de transportes não determinará um decréscimo da qualidade acústica do ambiente sonoro a que o Ser Humano se encontra sujeito no seu dia-a-dia.

Publicado em:
2ªs Jornadas de Engenharia Acústica "Responsabilidades e Desafios", Ordem dos Engenheiros, Lisboa, 2006 (comunicação oral).

ESTUDO DA SEQUÊNCIA SÍSMICA GERADA PELO SISMO DO FAIAL DE 9 DE JULHO DE 1998: ANISOTROPIA CRUSTAL, INVERSÃO TOMOGRÁFICA E CARACTERIZAÇÃO SISMO-TECTÓNICA

Afonso Dias, Nuno M.C.

Doutoramento em: Física, especialidade em Geofísica Interna
Grau Concedido por: Universidade de Lisboa
Orientadores: Luís Manuel H. Marques Matias e António A. R. Ribeiro
Provas Concluídas em: 17 de Março de 2006

O sismo de 9 de Julho de 1998 (M_L = 5,9) que atingiu as ilhas do Faial, Pico e São Jorge, nos Açores, iniciou uma crise sísmica de milhares de réplicas que se prolongou até ao início de 2005. A sua monitorização instrumental permitiu pela primeira vez um estudo aprofundado de uma crise sísmica nos Açores, em termos da caracterização da sismicidade e da estrutura crustal da região.

A distribuição da sismicidade indica que, das estruturas tectónicas principais existentes, a mais activa corresponde à de orientação NNW-SSE com desligamento esquerdo, com uma direcção secundária WSW-ENE de desligamento direito dominante. As estruturas NW-SE são confinantes da sismicidade.

Foi detectada a presença de anisotropia sísmica sob as estações sísmicas compatível com o modelo EDA, existindo correlação entre o índice de fracturação e o posicionamento de cada estação. A orientação estimada da direcção de compressão horizontal máxima indica um complexo padrão nas trajectórias da tensão com rotação da direcção NW-SE para SW-NE no sector oriental do Faial.

A inversão 1-D e 3-D indica que a crusta nos Açores, junto às ilhas do Faial e Pico, possui uma estrutura superficial heterogénea e uma crusta média-inferior bastante homogénea, situando-se a Moho a 12-13 km. O aumento de espessura em relação a uma crusta oceânica "típica" indica que a edificação crustal se deveu a uma elevada taxa de fornecimento magmático, que arrefeceu e cristalizou em profundidade sendo relativamente pouco importante a taxa de vulcanismo extrusivo. Foi detectada a presença de um volume com velocidades elevadas das ondas sísmicas, interpretada como a uma intrusão cristalina de rochas máficas e ultra-máficas, sendo também a assinatura clara das câmaras magmáticas sob os principais edifícios vulcânicos do Faial e Pico.

Agradecimentos: o autor beneficiou de apoio do programa PRODEP III, Medida 5, Acção 5.3 (Acções de Doutoramento).

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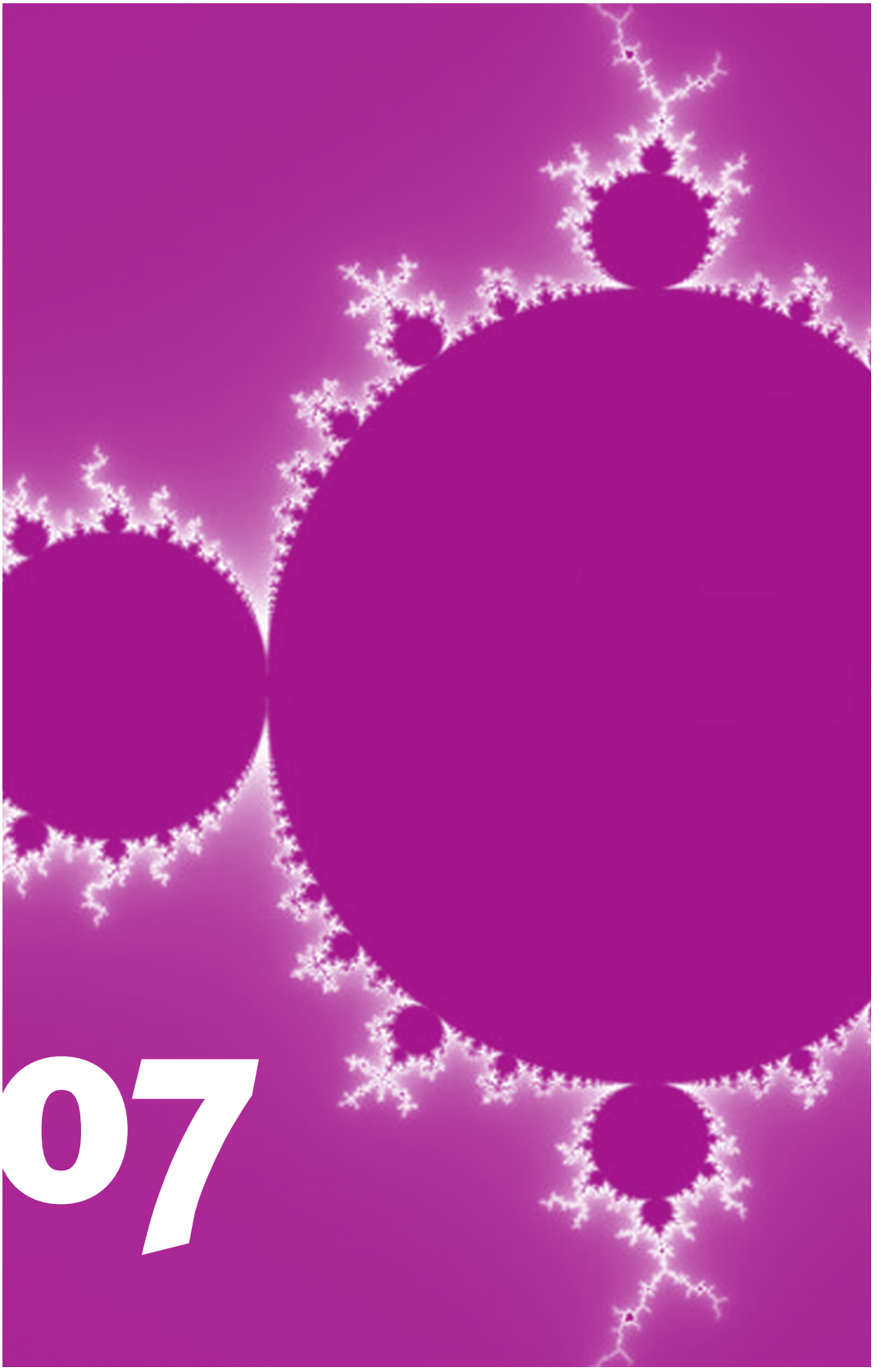
07

MATEMÁTICA

Anuário Científico 2006

ISEL

NUMERICAL SIMULATION OF AN OLDROYD-B FLUID WITH A PRECONDITIONED DOMAIN DECOMPOSITION METHOD

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This paper deals with the numerical implementation of a preconditioned domain decomposition method to approximate the solution of a non-Newtonian viscoelastic Oldroyd-B model. The governing equations can be decomposed into a Navier-Stokes system and a transport equation and a modified Schwarz scheme, involving block preconditioners for the Navier-Stokes equations, is used to solve iteratively the decoupled problems. Numerical results are provided for steady flow in the two-dimensional lid driven cavity.

Publicado em:
Proceedings of the 2006 IASME/WSEAS International Conference on Continuum Mechanics, Chalkida, Evia Island, Greece, pp. 97-102, 2006.

A PRECONDITIONED DOMAIN DECOMPOSITION METHOD FOR THE SIMULATION OF VISCOELASTIC FLOWS

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Publicado em:
WSEAS -Transactions on MATHEMATICS, issue 3, vol. 5, pp. 289-296, 2006.

In this paper we apply a domain decomposition method to approach the solution of a non-Newtonian viscoelastic Oldroyd-B model. The numerical scheme is based on a fixed-point argument applied to the original non-linear system of partial differential equations decoupled into a Navier-Stokes system and a tensorial transport equation. Using a modified Schwarz algorithm, involving block preconditioners for the Navier-Stokes equations, the decoupled problems are solved iteratively. Numerical simulations on a 4:1 abrupt contraction flow problem are considered to validate the scheme.

DISTRIBUIÇÃO DE CUSTOS DE COMPUTAÇÃO

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Em teoria da computação, um problema teórico e prático que tem vindo a ganhar crescente importância é o da maneira como se distribuem os custos de execução de algoritmos aplicados à resolução de problemas complexos. Esses custos podem ser medidos de diversos modos, nomeadamente em termos do tempo que o algoritmo demora até encontrar uma solução ou provar que nenhuma solução existe, ou por outra medida que se relacione com o tempo de execução do algoritmo mas que seja independente do computador onde este se executa. Em alguns problemas, nomeadamente problemas de satisfação de restrições (CSP - Constraint Satisfaction Problems), a distribuição dos custos de execução evidencia caudas pesadas, o que tem uma grande importância no estabelecimento de estratégias de recomeço de algoritmos aleatórios (restart strategies).
Neste trabalho mostram-se duas formas de gerar uma família que caracterize apropriadamente os custos de execução de certos algoritmos para diversos valores dos parâmetros do problema CSP. Nomeadamente, uma família de distribuições resultante da mistura de duas distribuições estáveis e uma resultante da soma de distribuições Erlang devidamente renormalizadas

Publicado em:
Actas do XIII Congresso Anual da SPE (2006), p. 249-256

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TYPES OF BIFURCATIONS OF FITZHUGH-NAGUMO

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The FitzHugh-Nagumo-like systems are of fundamental importance to the understanding of the qualitative nature of nerve impulse propagation. Our work provides a numerical investigation of bifurcations associated with a family of piecewise differentiable canonical maps for a planar FitzHugh-Nagumo system. We describe the bifurcation structure of the maps with the variation of the parameters.

Publicado em:
Nonlinear Dynamics, 44 (2006) 231-242

THE INFLUENCE OF COUPLING ON CHAOTIC MAPS MODELLING BURSTING CELLS

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Bursting behavior is ubiquitous in physical and biological systems, specially in neural cells where it plays an important role in information processing. This activity refers to a complex oscillation characterized by a slow alternation between spiking behavior and quiescence. In this paper, the interesting phenomena which transpire when two cells are coupled together, is studied in terms of symbolic dinamics. More specifically, we characterize the topological entropy of a map used to examine the role of coupling on identical bursters. The strength of coupling leads to the introduction of a second topological invariant that allows us to distinguish isentropic dynamics. We illustrate the significant effect of the strength parameter on the topological invariants with several numerical results.

Publicado em:
Chaos Solitons & Fractals, 28 (2006) 1314-1326

COMPUTATION OF THE TOPOLOGICAL ENTROPY IN CHAOTIC BIOPHYSICAL BURSTING MODELS FOR EXCITABLE CELLS

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Publicado em:
Discrete Dynamics in Nature and Society, (2006) 1-18

One of the interesting complex behaviors in many cell membranes is bursting, in which a rapid oscillatory state alternates with phases of relative quiescence. Although there is an elegant interpretation of many experimental results in terms of nonlinear dynamical systems, the dynamics of bursting models is not completely described. In the present paper we study the dynamical behavior of two specific three-variable models from the literature that replicate chaotic bursting. With results from symbolic dynamics, we characterize the topological entropy of one-dimensional maps that describe the salient dynamics on the attractors. The analysis of the variation of this important numerical invariant with the parameters of the systems, allows us to quantify the complexity of the phenomenon and to distinguish different chaotic scenarios. This work provides an example of how ourunderstanding of physiological models can be enhanced by the theory of dynamical systems.

LOW-DIMENSIONAL DYNAMICS OF CARDIAC ARRHYTHMIAS

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Strictly speaking, a cardiac arrhythmia is any departure of the heartbeat from strict periodicity. In that sense, all living persons have arrhythmias all the time, since the normal heartbeat is never exactly periodic. The study of cardiac arrhythmias, particularly those which are considered abnormal, is of great interest from a medical and mathematical perspective. They can be studied from the viewpoint of dynamical systems theory. We use the techniques of symbolic dynamics to study the topological entropy of a circle map that can be used to understand specific arrhythmias. Finally we introduce a second topological invariant to distinguish isentropic dynamics and we exhibit numerical results about maps with the same topological entropy. This work is still another illustration that our understanding of physiological models can be enhanced by the theory of dynamical systems.

Publicado em:
Proceedings of the European Conference on Iteration Theory (ECIT2004), August 29 - September 4, 2004, Batshuns, Austria, (2006), 55-68.

RADIAL SOLUTIONS FOR A NONLOCAL BOUNDARY VALUE PROBLEM

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We consider the boundary value problem for the nonlinear Poisson equation with a nonlocal term $\Delta u = f(u, \int_U g(u))$, $u|_{\partial U} = o$. We prove the existence of a positive radial solution when f grows linearly in u, using Krasnoselskii's fixed point theorem together with eigenvalue theory. In presence of upper and lower solutions, we consider monotone approximation to solutions.

Publicado em:
Boundary Value Problems Journal, Volume 2006 (2006) ID 32950

EVENNESS CONDITIONS FOR FOUR FACTORS CROSS NESTED MODELS

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Fonseca et al. (see [2]) obtained UMVUE for the variance components of balanced cross nested models. The estimators were the difference of a positive and a negative part. Unbiased estimators are obtained for the variance components of such models with cross-nesting. Following Michalski & Zmyslony (see [3]) we may use the quotient of the positive by the negative part of the estimators to test the nullity of the variance components. If either the degrees of freedom in the numerator or in the denominator are even we have, (see [1]) an exact expression for the distribution of the test statistic. It is thus interesting to see if this evenness conditions are a rarity or if they are satisfied in many circumstances. If we name as first evenness condition (1st) that all components of the vector g_1 are even and as second evenness condition (2nd) that all components of the vector g_2 are even, when at least one of these evenness conditions holds we have an exact expression for the distribution of the test statistic. We will answer this question for four factors models, showing that in more then half of the possible degrees of freedom combinations, at least one of the evenness conditions.

Publicado em:
Biometrical Letters 43, vol. 2 (2006), p. 109-130

A MODEL-BASED APPROACH TO INFORMATION RETRIEVAL SYSTEMS DEVELOPMENT

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We propose a novel model-based approach (MDA) for the design and creation of Information Retrieval (IR) systems. This is based on a specific language that provides common notation and concepts and a collaborative modular environment for the design of IR systems. The language is a UML profile, involving several stereotypes for the IR area. From this profile we derive standard libraries of modules that can be used in the development of IR systems. Through appropriate templates, we transform models into software code according different programming language and different IR platforms.

Publicado em:
Proceedings of Software Engineering and Applications (SEA 2006), 10th IASTED International Conference, November 13–15, 2006, Dallas, Texas, USA

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IRML – INFORMATION RETRIEVAL MODELING LANGUAGE

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We propose a specific language (created for the IR area) that provides a common notation and concepts for the design of IR systems. The language is based on UML extension mechanisms with specific stereotypes for IR. From this language (UML Profile) we define standard libraries of models and code templates that can be used in the development of IR systems. The main goal is to provide a novel approach that can guide the design of IR systems, using a common notation and concepts in a modular environment.

Publicado em:
Proceedings of Modelling, Simulation and Optimization (MSO 2006), 6th IASTED International Conference, 11-13 de Setembro 2006, Gaborone, Botswana

EIGENVALUES OF PRODUCTS OF MATRICES

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Publicado em:
Linear and Multilinear Algebra, vol. 54 (2006), 343-353.

Let A and B be nxn matrices over an algebraically closed fiel F. The pair (A,B) is said to be spectrally complete if, for every sequence c1,...,cn over F such that det(AB)=c1...cn, there exist nxn matrices A',B' over F similar to A,B, respectively, such that, A'B' has eigenvalues c1,...,cn. In this article, we described the spectrally complete pairs. Assuming that A and B are nonsingular, the possible eigenvalues of A'B', when A' and B' run over the sets of matrices similar to A and B, respectivelly, were described in a previous article.

CHAOTIC BEHAVIOR IN AN ECONOMIC MODEL

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The purpose of this work is to study a discrete-time nonlinear business cycle model of the Kaldor-type. The model is an extended Kaldor model and it is described by a two-dimensional dynamical system with income and capital as variables. We check the orbits of the system, their changes related to changes of the system parameters and their basins of attraction in order to understand the dynamic features of the model.

Publicado em:
Proceedings of the Workshop Perspectives on Econophysics, Universidade de Évora 2006, 99-109.

CHAOTIC BEHAVIOR IN A TWO-DIMENSIONAL BUSINESS CYCLE MODEL

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We consider a discrete-time economic model which is a particular case of the Kaldor-type business cycle model and it is described by a two-dimensional dynamical system. Under certain conditions the map can be reduced to a skew map whose components, the base and the fiber map, both have entropy. Our proposal is to study and measure the complexity of the system using symbolic dynamics techniques and the topological entropy.

Publicado em:
Proceedings of the Tenth International Conference on Difference Equations and Applications (ICDEA2005), Munich, Germany.

A SPACE OF GENERALIZED DISTRIBUTIONS

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In this paper we use a duality method to introduce a new space of generalized distributions. This method is exactly the same introduced by Schwartz for the distribution theory. Our space of generalized distributions contains all the Schwartz distributions and all the multipole series of physicists and is, in a certain sense, the smallest space containing all these series.

Publicado em:
Czechoslovak Mathematical Journal, 56 (131) (2006) 543-558

MULTIOBJECTIVE TOPOLOGY OPTIMIZATION OF STRUCTURES USING GENETIC ALGORITHMS WITH CHROMOSOME REPAIRING

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1 IDMEC-IST
2 DEETC-ISEL

Publicado em:
Springer, Structural and Multidisciplinary Optimization, Volume 32, Number 1, pp 31-3 Julho de 2006.

In this work, a genetic algorithm (GA) for multiobjective topology optimization of linear elastic structures is developed. Its purpose is to evolve an evenly distributed group of solutions to determine the optimum Pareto set for a given problem. The GA determines a set of solutions to be sorted by its domination properties and a filter is defined to retain the Pareto solutions. As an equality constraint on volume has to be enforced, all chromosomes used in the genetic GA must generate individuals with the same volume value; in the coding adopted, this means that they must preserve the same number of "ones" and, implicitly, the same number of "zeros" along the evolutionary process. It is thus necessary: (1) to define chromosomes satisfying this propriety and (2) to create corresponding crossover and mutation operators which preserve volume. Optimal solutions of each of the single-objective problems are introduced in the initial population to reduce computational effort and a repairing mechanism is developed to increase the number of admissible structures in the populations. Also, as the work of the external loads can be calculated independently for each individual, parallel processing was used in its evaluation. Numerical applications involving two and three objective functions in 2D and two objective functions in 3D are employed as tests for the computational model developed. Moreover, results obtained with and without chromosome repairing are compared.

GENERATION OF FEASIBLE MESHES FOR GA TOPOLOGY OPTIMIZATION OF STRUCTURES USING RANDOM KEYS

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1 IDMEC-IST
2 DEETC-ISEL

Topology optimization consists in finding the spatial distribution of a certain total mass of material in order for the resulting structure to have some optimal property, for instance, maximum stiffness. It is currently object of intense research. It is customary to initially discretize the continuum domain into finite elements (FE) and to define boundary conditions and applied loads to the resulting mesh. The optimization will consist in determining which elements will be present in the structure and which will be removed (voids).Since the usual genetic operators of crossover and mutation did not preserve the volume constraint and the selection pressure on infeasible individuals proved to be insufficient for their elimination in the course of the evolutionary process with the subsequent waste of computer time in evaluating infeasible designs, a repair mechanism was created to increase the number of feasible individuals in the population. In this paper we develop a method to generate initial feasible individuals that remain feasible upon crossover and mutation and as such do not require any repairing operator.

Publicado em:
6th ASMO-UK/ISSMO International Conference on Engineering Design Optimization. St Edmund Hall Oxford. July 2006.

POSITIVE DEFINITE MATRICES AND DIFFERENTIABLE REPRODUCING KERNEL INEQUALITIES

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Publicado em:
Journal of Mathematical Analysis and Applications 320 (2006), 279-292.

Let I be a real interval and $k: I^2 \to C$ be a reproducing kernel on I. By the Moore-Aronszajn theorem, every finite matrix $k(x_i,x_j)$ is positive semi-definite. We show that, as a direct algebraic consequence, if $k(x,y)$ is appropriatelly differentiable it satisfies a 2-parameter family of differential inequalities of which the classical diagonal dominance is the order o case. An application of these inequalities to kernels of positive integral operators yields optimal Sobolev norm bounds.

POSITIVE DEFINITE MATRICES AND INTEGRAL EQUATIONS ON UNBOUNDED DOMAINS

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The kernel of a continuous positive integral operator on an interval *I* is a Moore matrix on *I*. We show that, under minimal differentiability assumptions, this implies that the kernel satisfies a 2-parameter family of differential inequalities. These inequalities ensure that, for unbounded *I*, the corresponding integral operator is exceptionally well behaved: it is compact and thus the eigenfunctions for its discrete spectrum have the differentiability of the kernel and satisfy sharp Sobolev bounds, the symmetric mixed partial derivatives are again kernels of positive operators and the differentiated eigenfunction series converge uniformly and absolutely. Converse results are derived.

Publicado em:
Differential and Integral Equations 19, 2 (2006), 189-210.

EIGENVALUES OF POSITIVE DEFINITE INTEGRAL OPERATORS ON UNBOUNDED INTERVALS

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Publicado em:
Positivity(2006)Online First DOI 10.1007/ s11117-005-0040-z

Let $k(x,y)$ be the positive definite kernel of an integral operator on an unbounded real interval. If k belongs to class A defined below, the corresponding operator is compact and trace class. We establish two results relating smoothness of k and its decay rate at infinity along the diagonal with the decay rate of the eigenvalues. The first result deals with the Lipschitz case; the second deals with the uniformly C^1 case. The optimal results known for compact intervals are recovered as special cases, and the relevance of these results for Fourier transforms is pointed out.

INEQUALITIES FOR DIFFERENTIABLE REPRODUCING KERNELS AND AN APPLICATION TO POSITIVE INTEGRAL OPERATORS

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Let $I \subseteq \mathbb{R}$ be an interval and let $k: I^2 \to \mathbb{C}$ be a reproducing kernel on I. We show that if $k(x,y)$ is in the appropriate differentiability class, it satisfies a 2-parameter family of inequalities of which the classical diagonal dominance inequality for reproducing kernels is the o^{th} order case. We provide an application to integral operators: if k is a positive definite kernel on I (possibly unbounded) with differentiability class $S_n(I^2)$ and satisfies an extra integrability condition, we show that eigenfunctions are $C^n(I)$ and provide a bound for its Sobolev H^n norm. This bound is shown to be optimal.

Publicado em:
Journal of Inequalities and Applications Volume 2006, Article ID53743, 1-9.

A LINEAR ALGEBRAIC APPROACH TO HOLOMORPHIC REPRODUCING KERNELS IN CN

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Publicado em:
Linear Algebra and Applications 412(2006), 270-290.

Let $\Omega \subseteq C^n$ be a domain and k be a holomorphic reproducing kernel on Ω. By the Moore-Aronszajn characterization, every finite matrix $k(Z_i,Z_j)$ is positive semidefinite. We show that, as a direct algebraic consequence, $k(Z,U)$ satisfies an infinite 2n-parameter family of differential inequalities of which the classical diagonal dominance inequality for reproducing kernels is the order o case. In addition, the mixed hemisymmetric partial derivative of k with respect to any homologous variables yields again a holomorphic reproducing kernel on Ω. These results are interpreted in terms of the general theory of reproducing kernels.

EIGENVALUE DISTRIBUTION OF POSITIVE DEFINITE KERNELS ON UNBOUNDED DOMAINS

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We study eigenvalues of positive definite kernels of L^2 integral operators on unbounded real intervals. Under the assumptions of integrability and uniform continuity of the kernel on the diagonal the operator is compact and trace class. We establish sharp results which determine the eigenvalue distribution as a function of the smoothness of the kernel and its decay rate at infinity along the diagonal. The main result deals at once with all possible orders of differentiability and all possible rayes of decay of the kernel. The known optimal results for eigenvalue distribution of positive definite kernels in compact intervals are particular cases. These results depend critically on a 2-parameter differential family of inequalities for the kernel which is a consequence of positivity and is a differential generalization of diagonal dominance.

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ALGEBRAIC, DIFFERENTIAL, INTEGRAL AND SPECTRAL PROPERTIES OF MERCER-LIKE KERNELS

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We present a survey of recent results by the authors which show that reproducing kernels enjoy a closely knit of interplay of algebraic, differential, integral and spectral properties (whenever all are defined). The matrix characterization of reproducing kernels implies a family of differential dominance inequalities, which in turn acts as the appropriate integrability condition when these are kernels of L^2 integral operators. This fact allows complete and optimal determination of eigenvalue asymptotics.

ORIENTATIONAL DIRECTOR EFFECTS IN NEMATIC LIQUID CRYSTALS WITH SMALL ERICKSEN NUMBER

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Orientational director effects in nematic liquid crystals with small Ericksen number are investigated. The director field is disturbed by a semi-infinite plate on y = o and x $\leq$ U t and moving with a constant velocity U. Strong anchoring conditions at the plate are assumed. The resulting equations are a system of nonlinear partial differential equations for a nematic in the one elastic constant approximation. These equations are reduced to a coupled set of nonlinear ordinary differential equations by a suitable transformation. No such transformation seems possible for the many elastic constant case. The resulting equations are solved using analytical methods and strict bounding solutions obtained. These strict analytical solutions are compared with Picard iterated solutions.

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PLANAR MAGNETRON DISCHARGE. AN EXPERIMENTAL PROFILE ANALYSIS OF THE TARGET EROSION BASED ON A TWO-DIMENSIONAL FLUID MODEL IN THE STEADY STATE

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In the present work the erosion depth is measured along a diameter of a circular magnetron target. The horizontal and vertical components of the magnetic induction are measured at points of the plasma that are vertically above this diameter and at different distances from the target.

The experimental profile of the target erosion is analysed on the basis of the plasma density distribution near the target which is obtained using a two-dimensional fluid model in the steady state.

F AND SELECTIVE F TESTS WITH BALANCED CROSS-NESTING AND ASSOCIATED MODELS

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F tests and selective *F* tests for fixed effects part of balanced models with cross-nesting are derived. The effects of perturbations in the numerator and denominator of the *F* statistics are considered.

Balanced models with cross-nesting enable us to study the action of a large number of factors. Whenever possible, *F* tests are highly recommended due to their robustness and power.

In what follows such tests are derived for the fixed effects part of the models. Besides the usual *F* tests we will consider selective *F* tests which have higher power for chosen alternatives. Moreover, we consider the effects of perturbations on the numerator and denominator of the statistics. These perturbations arise when additional terms are added to the models, thus originating associated models.

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ELEARNING MATHEMATICS IN AN AFRICAN CONTEXT – AN INNOVATION CHALLENGE TOWARDS DEVELOPMENT

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In this paper we begin by explaining the importance of information and communication technologies – with special relevance to e-learning as factors of the information society the world is giving birth. Next, recognizing the digital divide and the development gap existing between rich and poor countries, we show the importance of ICT and e-learning in Africa as a part of the making of African innovation systems. Afterwards, Mathematics is briefly presented in its past, present and future as one of the greatest achievements and adventures of human history: it has always been related with culture through theoretical developments and practical applications. In our information society it is a fundamental discipline in the basis of most technological and societal devices.

We then present 2AMAC as an e-learning project on Mathematics, which is yet a work on progress made at ISEL. It is considered as a tool to improve and complement our teaching, designed to motivate students to the importance of Analysis Mathematics to the formation of an engineer. We are opened to cooperation, so 2AMAC might also contribute to the formation of engineers in African countries (mainly those with official Portuguese language).

We conclude recognizing the complexity and interrelationship that exist in the global world we are living in. In universities, engineering plays and important role in establishing conditions towards sustainable development at a global and local scale. With our project we hope to give a small contribute to the achievement of the Millenium Goals maybe in countries where they are most far away. We also want to learn and change experiences with African innovation systems.

COMPUTING CONDITIONALLY INVARIANT MEASURES AND ESCAPE RATES

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We consider expanding discontinuous maps with holes and the associated Markov partitions. These partitions are characterized by the orbits of the turning points and the discontinuity points of the maps. For these maps we study the process of escape of points from the interval, that is characterized by a conditionally invariant measure. We construct this measure which naturally generates an unique invariant probability measure. A direct consequence of these results is to compute explicitly the escape rate, with connection to the transfer operator. We also introduce a weighted kneading theory which allows a rigorous computation of the escape rate.

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A THREE-FIELD NONCONFORMING MULTIDOMAINS METHOD FOR CONTACT PROBLEMS

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With this work we present nonconforming finite elements approximation of the contact problem based on a three-fields multidomains formulation. We will show for some examples that the numerical results obtained with nonconforming multidomains techniques are qualitatively equivalent to the classic results and quite better than the standard mortar method.

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METODOLOGIA PARA A CONCEPÇÃO DE SISTEMAS DE RECUPERAÇÃO DE INFORMAÇÃO

Ferreira, João Carlos Amaro

Propõe-se nesta dissertação uma metodologia para a concepção e construção de sistemas de IR, em particular no contexto do espaço distribuído e descentralizado que é a Web. Esta metodologia inclui uma linguagem de modelação (IRML-Information Retrieval Modelling Language), e baseada no mecanismo de extensão do UML e adequada às necessidades da Recuperação de Informação (IR). Para facilitar o processo de construção e promover a colaboração entre os investigadores de IR, é proposto um conjunto de bibliotecas padrão baseadas na linguagem IRML, no qual está embebido os principais conceitos da IR. Destas actividades resulta um conjunto de sistemas conceptuais que são implementados usando uma infra-estrutura adequada. Este conjunto de etapas permite simplificar o processo de construção de sistemas de IR. São construídos dez sistemas de IR ao qual se junta uma plataforma de teste onde são testados mais de mil sistemas num ambiente controlado. Esta plataforma permite testar processos existentes e outros construídos de raiz, nomeadamente novos processos de comparação híbridos, novas fórmulas de seguimento de ligação, pseudo-retroacção e de combinação de resultados.

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ON THE ALGEBRAIC, DIFFERENTIAL, INTEGRAL AND SPECTRAL PROPERTIES OF MERCER-LIKE KERNELS

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Instituto Superior Técnico, Universidade Técnica de Lisboa, Tese de Doutoramento em Matemática, Lisboa, Portugal, Janeiro de 2006

Suppose E is an interval in R or a domain in C^n and k a reproducing kernel (or Moore matrix) on E. Then, as a direct algebraic consequence, we show that, if $k(x,y)$ is appropriately differentiable, it satisfies a 2-parameter family of differential inequalities of which the classical diagonal dominance is the order o case [1], [2].

We show that a Mercer-like kernel on a (possibly unbounded) real interval I is a reproducing kernel and the kernel of a positive, compact, trace class operator K in $L^2(I)$. As a consequence of the differential inequalities, the eigenfunctions have the differentiability of the kernel, the corresponding series converge absolutely and uniformly and may be differentiated term by term. Under additional conditions, symmetric mixed partial derivatives are again Mercer-like kernels satisfying sharp Sobolev bounds and the differentiated eigenfunction series converge uniformly and absolutely. Converse results are derived [1], [3], [4].

We establish sharp estimations of the eigenvalue distribution of K as a function of the smoothness of the kernel and its decay rate at infinity along the diagonal which generalize optimal results known for the case where I is compact, [5], [6].

If $k^{1/2}(x,x)$ is in $L^1(R)$, we show that all these results are carried through to a "rotated" Fourier transform, which preserves the spectrum and trace of the associated operators, [3], [6].

ANÁLISE CONJUNTA DE REGRESSÕES E PLANOS DE MELHORAMENTO

Pinto, Iola

A Análise Conjunta de Regressões, ACR, é uma técnica conhecida pela sua utilização na comparação e selecção de cultivares. A sua aplicação estava geralmente condicionada a ensaios realizados num número reduzido de anos, para um conjunto fixo de cultivares. Neste trabalho, estuda-se a extensão do âmbito de aplicação desta técnica a planos de melhoramento. Numa primeira parte, serão apresentadas as técnicas estatísticas que serão utilizadas posteriormente na análise dum plano de melhoramento concreto. Mostra-se nomeadamente, como realizar os ajustamentos das regressões lineares, como fazer inferência estatística e como proceder à comparação, classificação e selecção dos cultivares.

Na segunda parte deste trabalho mostra-se, revendo-nos no Plano de Melhoramento de Trigo Mole em Portugal (1986 - 2000), como utilizar a ACR em planos de melhoramento.

Será ainda apresentado um modelo para explicar os índices ambientais, usando variáveis dummy associadas a anos, locais e cultivares. Os coeficientes ajustados para os anos foram usados para expressar, no caso do Programa de Melhoramento do Trigo Mole em Portugal, os efeitos atribuíveis ao factor ano.

Os resultados obtidos no caso Português, indicam claramente a utilidade da técnica da ACR no acompanhamento de programas de melhoramento, mais precisamente, na tomada de decisão relativa aos cultivares que devem permanecer no plano de melhoramento de um ano para o outro.

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DINAMICA DE MODELOS COSMOLÓGICOS

Azevedo, Tiago Charters de

Editado por:
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Nesta tese apresenta-se o estudo da relaxação de vários modelos cosmológicos para o comportamento inflacionário de de Sitter através da construção de funções de Liapunov, da dinâmica do universo na presença e combinação de três componentes materiais e da dinâmica do mecanismo de reaquecimento do universo através do decaimento do inflatão num campo escalar através de ressonância paramétrica.
Começa-se por uma introdução no Capítulo 1 com o objectivo de fixar notação e algumas definições.
No Capítulo 2 estuda-se a relaxação de vários modelos cosmológicos para o comportamento inflacionário de de Sitter através da construção de funções de Liapunov como alternativa à aproximação linear. Os resultados são na sua maioria conhecidos, mas o método apresentado, baseado na construção de uma função de Liapunov, dá informação adicional em relação aos métodos da aproximação linear usados na literatura.
A dinâmica do universo na presença de dois fluidos em interacção é estudada no Capítulo 3. Mostra-se a existência de soluções de \emph {scaling} para diversos valores dos parâmetros dos fluidos e dos termos de interacção. Discute-se também o comportamento inflacionário das soluções e os constrangimentos impostos pela núcleosíntese ao acoplamento considerado.
O Capítulo 4 descreve a teoria de reaquecimento do universo através do decaimento do inflatão num campo escalar com ressonância paramétrica. No regime *narrow resonant* mostra-se, num espaço-tempo de Minkowski, como reduzir a equação do movimento para os modos do campo escalar a uma equação de Hill. Estuda-se também o mecanismo de reaquecimento num universo em expansão. No regime *broad resonant* a dinâmica no espaço-tempo de Minkowski pode ser usada para obter o número de partículas produzidas num universo em expansão durante o primeiro período de *preheating*. Faz-se um estudo sistemático da duração deste regime em função do acoplamento entre os campos escalares.

COMPORTAMENTO CAÓTICO EM SISTEMAS FISIOLÓGICOS

Duarte, Jorge

Neste trabalho estudamos a dinâmica de modelos biofísicos caóticos que representam a actividade eléctrica de células excitáveis.
Usando técnicas da teoria dos sistemas dinâmicos, quantificamos a complexidade das estruturas fisiológicas através da análise de determinadas aplicações no intervalo. Mais precisamente, caracterizamos a entropia topológica e um segundo invariante topológico, denotado por r, com o propósito de descrever o comportamento caótico dos modelos.
Primeiramente, apresentamos um estudo da dinâmica de um modelo do tipo FitzHugh-Nagumo submetido a um estímulo periódico.
No contexto dos ritmos fisiológicos, proporcionamos uma caracterização da dinâmica de uma família de aplicações na circunferência que foi proposta como modelo para osciladores não lineares periodicamente forçados.
Atendendo à sua importância, analisamos modelos biofísicos para o comportamento "explosivo" de células excitáveis. A dinâmica de uma célula singular e a caracterização do efeito de acoplamento em células "explosivas" idênticas, é particularmente interessante para o nosso estudo.
Finalmente, apresentamos algumas considerações sobre a relevância do comportamento caótico em sistemas neuronais como factor crucial de adaptação a um meio em constante evolução.

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ALGUNS PROBLEMAS DE FACTORIZAÇÃO DE MATRIZES

Charters de Azevedo, Laura Cristina Teixeira Iglésias

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Os problemas estudados nesta dissertação inserem-se nos seguintes problemas de factorização de matrizes:
Em que condições é possível escrever uma matriz como produto de duas matrizes com certas condições invariantes por semelhança prescritas?
Em que condições o produto de duas matrizes com classes de semelhança prescritas, pode satisfazer certas condições invariantes por semelhança prescritas? As matrizes estudadas são quadradas e com entradas num corpo. No primeiro capítulo, apresentam-se conceitos e resultados que são utilizados ao longo da dissertação. Apresentam-se também os problemas estudados e vários resultados que serviram de motivação a estes problemas. No segundo capítulo, estudam-se condições necessárias e suficientes para que uma matriz se escreva como produto de duas matrizes com características e valores próprios prescritos. No terceiro capítulo, estuda-se em que condições uma matriz quadrada sobre o corpo dos números reais é produto de duas matrizes com polinómios característicos prescritos. Vários lemas que facilitam a realização deste estudo são demonstrados num corpo arbitrário. No quarto capítulo, estudam-se os possíveis valores próprios do produto de duas matrizes com classes de semelhança prescritas, num corpo F algebricamente fechado. Um par de matrizes (A, B) do tipo $n \times n$ sobre F diz-se espectralmente completo se, para qualquer sequência $c_1, \ldots, c_n$ de elementos de F tais que $c_1 \ldots c_n$ é igual ao determinante de AB, existem matrizes A', B' do tipo $n \times n$ sobre F, semelhantes a A, B, respectivamente, tais que AB tem valores próprios $c_1 \ldots c_n$. No quarto capítulo, identificam-se os pares de matrizes sobre F espectralmente completos.

COMPLETAÇÃO DE MATRIZES REAIS

Teixeira de Matos, Isabel Maria

Seja F um corpo. Em 1975, G.N. de Oliveira propôs o seguinte conjunto de problemas de completação de matrizes: descrever os possíveis polinómios característicos de uma matriz A quadrada de ordem *n*, particionada em quatro blocos, sendo dois deles principais e quadrados de ordens *p* e *q*, com *p*+*q*=*n*, quando alguns dos blocos estão fixos e os restantes variam.
Somente alguns deles, aqueles que correspondem à prescrição de uma submatriz de *A*, estão foram completamente resolvidos. Os outros foram resolvidos em casos particulares.
Nesta tese, estudam-se dois desses problemas sobre o corpo dos números reais. No primeiro, correspondente à prescrição dos dois blocos não principais, mostra-se que existe sempre uma completação de *A*, excepto quando o polinómio característico não admite um divisor de grau p e um dos blocos prescritos é nulo. O estudo do segundo, aquele em que são fixados os blocos principais, é decomposto na abordagem de duas situações:
- Pelo menos uma das matrizes prescritas é não escalar;
- Ambas as matrizes prescritas são escalares.

Em ambas, são estabelecidas condições para a existência de uma completação de *A*. Uma delas comum – a condição de traço – outra com uma característica comum – a exigência de uma certa factorização do polinómio característico.

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DOMAIN DECOMPOSITION METHODS FOR NON-NEWTONIAN FLUIDS

Borges, L.

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Instituto Superior Técnico, Universidade Técnica de Lisboa, Tese de Doutoramento em Matemática, Lisboa, Portugal, Dezembro de 2006.

The aim of this thesis is to study the numerical implementation of a preconditioned domain decomposition method applied to the finite element approximation of steady flows of non-Newtonian viscoelastic Oldroyd-B fluids. The constitutive equations of the model problem lead to a non-linear system of partial differential equations of mixed type that can be decoupled into a Navier-Stokes system and a tensorial transport equation. A modified Schwarz scheme, involving block preconditioners for the Navier-Stokes equations, is used to solve iteratively the two decoupled problems. The preconditioned domain decomposition method is applied to two well known benchmark flow problems, the lid driven cavity and the 4:1 abrupt planar contraction, to validate the numerical scheme. The method is also applied to a bifurcating channel and the corresponding numerical results are analyzed. Finally, the more general case of generalized Oldroyd-B flows in a curved pipe is considered, and numerical results are obtained for certain values of the rheological parameters, using the preconditioned domain decomposition method.

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