ANUÁRIO CIENTÍFICO 2008

Resumos de Artigos, Comunicações, Teses e Livros

INSTITUTO SUPERIOR DE ENGENHARIA DE LISBOA

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NOTA INTRODUTÓRIA

A divulgação do conhecimento resultante da Ciência, Investigação e Actividade Profissional de mérito reconhecido são indissociáveis e necessários numa sociedade em evolução, sem descurar a vertente pedagógica, numa Instituição de Ensino Superior.
Verificou-se que durante este período se assistiu a um incremento das publicações científicas dos docentes do ISEL. Por outro lado, existiu um maior envolvimento em projectos de investigação e um acréscimo na conclusão do grau de Doutor.
Assim, o anuário científico de 2008 constitui um documento de divulgação desta actividade no Instituto Superior de Engenharia de Lisboa em parceria com outros Politécnicos, Universidades e Centros de Investigação nacionais e internacionais.
Numa altura em que se avizinham mudanças estruturais no Ensino Superior, esperamos que o poder político avalie as instituições pelo trabalho desenvolvido e pela qualidade dos engenheiros que estas formam.

O Presidente do Conselho Científico

(Prof. José A. Paixão Coelho)

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ISEL

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ENGENHARIA CIVIL

Anuário Científico 2008

ISEL

SUSTAINABLE WATER REUSE IN PORTUGAL

Marecos do Monte, Maria Helena F.

Departamento de Engenharia Civil, ISEL, Lisboa, Portugal

Portugal, like most of Mediterranean EU member states, regularly experience severe water supply and demand imbalances, particularly in the summer months. Half of Portugal mainland suffers of water deficit. Tourism is a very important economic activity in Portugal and is pushing water demand particularly in regions suffering of water deficit, like the Algarve. Golf courses are an important tourist factor contributing to water demand rising. A number of golf courses are installed in tourist areas and need high amount of water for irrigation. Water reuse is a very important management strategy in situations of water scarcity. Portugal badly needs to include treated wastewater as a dependable water in the nation water resources management. Safe water reuse requires guidelines. This standard presents guidelines on: water quality, irrigation practice, management of environmental impacts, protection of public and animal health and aspects of control and monitoring.

Publicado em:
WSEAS Transactions on Environment and Development, 9(4):716-724, Set 2008.

FROM UNTHINNED CONTINENT TO OCEAN: THE DEEP STRUCTURE OF THE WEST IBERIA PASSIVE CONTINENTAL MARGIN AT 38°N

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Publicado em:
Tectonophysics, 2008, 458 , 9-50

The crustal and lithospheric mantle structure at the south segment of the west Iberian margin was investigated along a 370 km long seismic transect. The transect goes from unthinned continental crust onshore to oceanic crust, crossing the ocean–continent transition (OCT) zone. The wide-angle data set includes recordings from 6 OBSs and 2 inland seismic stations. Kinematic and dynamic modeling provided a 2D velocity model that proved to be consistent with the modeled free-air anomaly data. The interpretation of coincident multi-channel near-vertical and wide-angle reflection data sets allowed the identification of four main crustal domains: (i) continental (east of 9.4°W); (ii) continental thinning (9.4°W–9.7°W); (iii) transitional (9.7°W–_ 10.5°W); and (iv) oceanic (west of _ 10.5°W). In the continental domain the complete crustal section of slightly thinned continental crust is present. The upper (UCC, 5.1–6.0 km/s) and the lower continental crust (LCC, 6.9–7.2 km/s) are seismically reflective and have intermediate to low P-wave velocity gradients. The middle continental crust (MCC, 6.35–6.45 km/s) is generally unreflective with low velocity gradient. The main thinning of the continental crust occurs in the thinning domain by attenuation of the UCC and the LCC. Major thinning of the MCC starts to the west of the LCC pinchout point, where it rests directly upon the mantle. In the thinning domain the Moho slope is at least 13° and the continental crust thickness decreases seaward from 22 to 11 km over a _ 35 km distance, stretched by a factor of 1.5 to 3. In the oceanic domain a two-layer high-gradient igneous crust (5.3–6.0 km/s; 6.5–7.4 km/s) was modeled. The intra-crustal interface correlates with prominent mid-basement, 10–15 km long reflections in the multi-channel seismic profile. Strong secondary reflected PmP phases require a first order discontinuity at the Moho. The sedimentary cover can be as thick as 5 km and the igneous crustal thickness varies from 4 to 11 km in the west, where the profile reaches the Madeira-Tore Rise. In the transitional domain the crust has a complex structure that varies both horizontally and vertically. Beneath the continental slope it includes exhumed continental crust (6.15–6.45 km/s). Strong diffractions were modeled to originate at the lower interface of this layer. The western segment of this transitional domain is

highly reflective at all levels, probably due to dykes and sills, according to the high apparent susceptibility and density modeled at this location. Sub-Moho mantle velocity is found to be 8.0 km/s, but velocities smaller than 8.0 km/s confined to short segments are not excluded by the data. Strong P-wave wide-angle reflections are modeled to originate at depth of 20 km within the lithospheric mantle, under the eastern segment of the oceanic domain, or even deeper at the transitional domain, suggesting a layered structure for the lithospheric mantle. Both interface depths and velocities of the continental section are in good agreement to the conjugate Newfoundland margin. A < 40 km wide OCT having a geophysical signature distinct from the OCT to the north favors a two pulse continental breakup.

ON THE FOCAL MECHANISM OF THE 26.05.1975 NORTH ATLANTIC EVENT; CONTRIBUTION FROM TSUNAMI MODELLING

Kaabouben, F.[1]; Ibn Brahim, A.[2]; Toto, E.A.[1]; Baptista, M.A.[3,4]; Miranda, J.M.[4]; Soares, P.[3,4]; Luis, J.F.[5]

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Publicado em:
Journal of Seismology, doi 10.1007/s10950-008-9110-6, 2008.

The 1975 May 26 earthquake, of magnitude Ms=7.9, occurred in the North Atlantic, close to the Azores Archipelago. Its epicentre, as given by the US Geological Survey, was 17.5ºW, 35.9ºN, 200 km south of the Gloria Fault. Several authors determined the focal mechanism as a dextral strike-slip event with no significant dip-slip component, compatible with the relative motion between Eurasia and Nubia plates but away from the preseukmed plate boundary. The 1975 earthquake generated a tsunami of small amplitude recorded at the Portuguese tide-gage network, in Spain and Northern Africa. The peculiar location of the earthquake and tsunami source and the generation of a noticeable tsunami were already discussed by several authors, but up to now, no direct modelling of the tsunami generation and propagation was made to judge the set of source solutions obtained by sesimological analysis. In this paper we present the tsunami simulations, backward ray tracing and forward non linear shallow water simulations using data from Iberia and Azores and northern Africa. We show that a good fit between observed data and synthetic waveforms can be obtained with a focal mechanism with no significant dip-slip component, favouring its interpretation as almost pure dextral strike slip event located in an old fracture zone south of Gloria Fault.

THE TWO FACES OF THE REDLICH–KISTER EQUATION AND THE LIMITING PARTIAL MOLAR VOLUME OF WATER IN 1-AMINOPROPAN-2-OL

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The properties of the Redlich–Kister equation when expressed in power series of x_1 - x_2 are related to its alternative expression in terms of power series of x_2 - x_1, where x_1 and x_2 are mole fractions of the components 1 and 2 of a binary liquid mixture. The simple relationship between both sets of coefficients is derived and shown to conceal pitfalls while using Redlich–Kister coefficients to estimate partial molar properties of the components. The zero-powered terms, which are the same for the alternative expansions, are shown to yield a quarter of the excess molar property for the equimolar mixture. Literature data for the partial molar volume of water at infinite dilution in 15 neat aminoalkanols at different temperatures are collected and tabulated. These data generally show a positive dependence of that limiting value on the temperature, the only apparent exception being in the case of 1-aminopropan-2-ol. It is demonstrated that the recently published data for this aminoalkanol (Thermochim. Acta 440 (2006) 122) were ill-treated and recalculated limiting values are given, which increase with increasing temperature.

Publicado em:
Thermochimica Acta 468 (2008) 119-123.

01

REFORÇO SÍSMICO EM CONSTRUÇÕES EM TERRA CRUA

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Publicado em:
Revista Engenharia e Vida - Engenharia Civil, Construção e Desenvolvimento, 2008, 46, 46-52.

Pretende-se, com este artigo, descrever os principais tipos de reforço (horizontal e vertical) nas construções de terra crua, verificando a exequibilidade destas soluções. Uma vez que as construções de terra apresentam uma resposta muito negativa face a acção sísmica, é importante reforçar estas estruturas de modo a que possam resistir a um sismo sem danos graves. Verifica-se, assim, que uma correcta abordagem no tipo de reforço a utilizar-se minimiza os efeitos negativos da acção sísmica.

CONCEPÇÃO DE CONSTRUÇÕES EM TERRA CRUA - ZONAS SÍSMICAS (PARTE I)

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Neste artigo, baseado na dissertação de mestrado do primeiro autor (Gomes, 2008) e dedicado à construção sismo-resistente em terra crua, após uma primeira descrição do estado da arte a nível mundial e em particular, em Portugal. Analisa-se este tipo de construções em zonas sísmicas, verificando que estas apresentam uma resposta negativa quando sujeitas à acção sísmica. São ilustradas as soluções ideais de geometrias neste tipo de edificações, recomendadas por especialistas da área, estando estas localizadas em zonas sísmicas. Verifica-se assim, que uma correcta abordagem das dimensões na altura do projecto minimiza os efeitos negativos da acção sísmica.

Publicado em:
Revista Arquitectura e Vida, 2008, 95, 86-89.

CONCEPÇÃO DE CONSTRUÇÕES EM TERRA CRUA - ZONAS SÍSMICAS (PARTE II)

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Publicado em:
Revista Arquitectura e Vida, 2008, 96, 84-87.

Neste artigo, baseado na dissertação de mestrado do primeiro autor (Gomes, 2008) e dedicado à construção sismo-resistente em terra crua, após uma primeira descrição do estado da arte a nível mundial e em particular, em Portugal. Analisa-se este tipo de construções em zonas sísmicas, verificando que estas apresentam uma resposta negativa quando sujeitas à acção sísmica. São ilustradas as soluções ideais de geometrias neste tipo de edificações, recomendadas por especialistas da área, estando estas localizadas em zonas sísmicas. Verifica-se assim, que uma correcta abordagem das dimensões na altura do projecto minimiza os efeitos negativos da acção sísmica.

EARTH CONSTRUCTION STRENGTHENED WITH REINFORCED CONCRETE FRAMES

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In this paper, based on the Masters dissertation of the first author Gomes [5] and dedicated to seism-resistant earth construction, after a short introduction a building strengthened with reinforced concrete frames subjected to a seismic action is analyzed in terms of its dynamic characteristics and maximum displacements and stresses, which are compared with admissible values. In this analysis a three-dimensional structural model was used the software SAP 2000 (Structural Analysis Program), version 10.0.1. The objective is to fully understand the effect of a seismic action on this type of buildings strengthened with reinforced concrete.

Publicado em:
Revista estrangeira electrónica Teoria e Prática na Engenharia Civil, 2008, 12, Volume 8, 37-47.

01

A REUTILIZAÇÃO DE ÁGUAS RESIDUAIS TRATADAS E A GESTÃO SUSTENTÁVEL DOS RECURSOS HÍDRICOS

Marecos do Monte, Maria Helena F.

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Publicado em:
A Engenharia pelo Combate à Pobreza, pelo Desenvolvimento e Competitividade, CLME'200- II CEM, Maputo, Editado por J.F. Silva Gomes e tal, pp. 329-330.

A disponibilidade de recursos hídricos reflecte a sazonalidade climática. As necessidades de água para as actividades humanas também não são constantes ao longo do tempo: alguns factores, como o crescimento populacional, a crescente urbanização, o desenvolvimento industrial e a agricultura, induzem um permanente aumento das necessidades de água; outros factores determinam aumento sazonais de necessidade de água, coincidindo, frequentemente, esse aumento com períodos de baixa precipitação atmosférica e de elevada evaporação, como são exemplo a agricultura e o turismo (que determina elevado crescimento de população num prazo muito curto). Tais situações podem originar sérios desequilíbrios entre necessidades e disponibilidades de água, que podem atingir níveis graves em anos anormais de escassa precipitação. A degradação da qualidade das águas naturais decorrente de insuficiente controlo da poluição de origem antropogénica introduz limitações ao aproveitamento de alguns recursos hídricos, acentuando os desequilíbrios quantitativos entre a procura e a disponibilidade de água. Aos problemas de disponibilidade de água, em quantidade e em qualidade suficientes à satisfação das necessidades, juntam-se as consequências das alterações climáticas. Tanto as secas como as cheias anunciadas como prováveis consequências das alterações climáticas concorrem para menor disponibilidade água em quantidade, no caso das secas e de qualidade, no caso das cheias.

A gestão dos recursos hídricos emerge assim, já no início do século XXI, como um dos paradigmas da sustentabilidade do desenvolvimento socio-económico. O desenvolvimento tecnológico traz resposta a algumas questões de desenvolvimento dos recursos hídricos, como por exemplo, através da construção de grandes barragens ou a dessalinização de água do mar, mas não é suficiente para assegurar a sustentabilidade da gestão desses recursos. Torna-se necessária a concomitante adopção de outras estratégias, com o objectivo de conservar os recursos hídricos existentes, como sejam a implementação de medidas de uso mais eficiente da água, como a reutilização da água. Esta última estratégia – reutilização da água para fins múltiplos – tem

emergido nos últimos anos, de forma enfática, como um paradigma da sustentabilidade da gestão dos recursos hídricos.
O desenvolvimento da reutilização da água tem sido impulsionado pela escassez de água. No entanto, mais recentemente, a reutilização também sido desenvolvida como uma solução alternativa às crescentes exigências dos requisitos de licenciamento de descarga dos efluentes nos meios receptores.
Planear e executar com sucesso um projecto de reutilização de água requer que sejam satisfeitos três princípios: (1) assegurar que o tratamento das águas residuais se processa por meio de operações e processos fiáveis para a produção de um efluente que satisfaça os requisitos de qualidade compatíveis com a utilização pretendida; (2) assegurar a protecção da saúde pública; (3) ganhar a aceitação pública.
Os principais tipos de utilização de águas residuais tratadas são, por ordem decrescente de volume reutilizado, as seguintes: rega agrícola, rega paisagística, abastecimento industrial, recarga de aquíferos, usos ambientais e recreativos, usos urbanos não potáveis e indirecta ou directamente para abastecimento potável.
Na maioria das aplicações de reutilização os riscos sanitários e ambientais são considerados praticamente inexistentes, porque controlados adequadamente. A presença de alguns constituintes nos efluentes representa mesmo um benefício para certas utilizações. O exemplo mais característico é a fertilização proporcionada pela reutilização de águas residuais para rega, devido ao conteúdo das águas residuais em azoto e fósforo. O desenvolvimento tecnológico actual possibilita até que a partir de águas residuais se produza água adequada ao consumo humano. Porém, do ponto de vista de reutilização da água, não interessa propriamente o nível de tratamento das águas residuais na ETAR, mas a qualidade da água a reutilizar, no sentido de ser adequada à utilização pretendida e de não potenciar riscos de saúde pública nem impactes ambientais adversos. Assim, dependendo da aplicação de reutilização, poderá ser apropriado recorrer a processos de tratamento de "baixa" tecnologia, como lagoas de estabilização, como a processos de elevada complexidade tecnológica, como as tecnologias de membrana.
Neste trabalho apresentam-se os aspectos de qualidade que as águas residuais tratadas devem satisfazer antes de serem reutilizadas e caracterizam-se as soluções tecnológicas disponíveis, em termos de eficiência, custos e condições de operacionalidade.

ÁGUAS RESIDUAIS TRATADAS: RECURSO HÍDRICO ALTERNATIVO NO ÂMBITO DA UTILIZAÇÃO SUSTENTÁVEL DA ÁGUA EM PORTUGAL

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Publicado em:
Anuário da Água, 146/38-41, Jan 2008.

Mais de metade do território de Portugal continental apresenta um défice hídrico, principalmente as regiões localizadas no interior leste e a sul da bacia do Tejo. O período de déficite hídrico tem impactes agravados por outros factores, como a sua coincidência temporal com o aumento das necessidades de água para algumas actividades de elevado valor económico, de entre as quais se destaca a agricultura e o turismo.

Segundo os dados do Plano Nacional da Água (INAG, 2001), a agricultura é, de longe, maior consumidor de água, com 87,3% do consumo total. O turismo tem registado elevado desenvolvimento em Portugal nas últimas três décadas e representa uma fatia do PIB da ordem de 8% (ICEP, 2007). Portugal ocupa o 19º lugar entre os principais destinos turísticos e o 21º no que se refere a receitas. O turismo altera sazonalmente a composição demográfica das zonas turísticas, chegando a provocar a duplicação da população num prazo muito curto, de 2 a 3 meses. Actualmente, no nosso país o turismo encontra-se associado à instalação de campos de golfe em algumas regiões, designadamente no Algarve.

Desta breve caracterização da situação ressalta como evidente que o desenvolvimento sócio-económico de Portugal passa pela gestão sustentável dos recursos hídricos nacionais. A evolução temporal das disponibilidades de água, das necessidades e dos consumos e respectivas relações, avaliados em termos médios de Portugal continental, indica que, enquanto as disponibilidades hídricas se manterão praticamente constantes, as necessidades e os consumos tendem a crescer moderadamente, para satisfazer as exigências do desenvolvimento sócio-económico, podendo eventualmente, vir a estabilizar dentro de um horizonte de médio prazo. O desenvolvimento dos recursos hídricos em Portugal já não poderá assentar essencialmente nos rios e nos aquíferos menos profundos, de mais fácil acesso, os quais já se encontram largamente aproveitados. Torna-se assim mais evidente a necessidade de desenvolvimento de origens de água alternativas para satisfação do rápido crescimento das necessidades. Com este objectivo de desenvolvimento de origens de água alternativas

pode considerar-se um conjunto de estratégias, entre as quais se salienta a reutilização da água para múltiplos usos.
O desenvolvimento da reutilização da água tem sido impulsionado pela escassez de água. No entanto, mais recentemente, a reutilização também sido desenvolvida mesmo em regiões sem problemas de recursos hídricos, por motivos ambientais. Efectivamente, ao recuperar a água, através do tratamento das águas residuais, para uma posterior utilização, cumprem-se duas funções de protecção ambiental: (1) o efluente não é descarregado num meio receptor, assim se reduzindo a carga poluidora sobra as águas superficiais e subterrâneas; (2) o efluente tratado é utilizado como uma origem de água para abastecimento de uma determinada utilização.
Algumas aplicações de reutilização de água podem requerer uma afinação complementar das características típicas de efluentes secundários e terciários. Actualmente, é possível produzir água com características compatíveis com qualquer utilização, dada a bastante vasta panóplia de operações e processos unitários que se podem considerar para tratamento de águas residuais consoante os poluentes cuja remoção é pretendida. É indispensável salientar que, para assegurar a protecção da saúde pública, sem desnecessariamente desencorajar a reutilização da água, não basta tratar as águas residuais até aos níveis de qualidade compatíveis com as finalidades de reutilização, mas é essencial planear medidas de minimização da exposição dos seres humanos às águas reutilizadas e garantir a fiabilidade da solução, avaliada através da monitorização da sua execução prática.
A reutilização de águas residuais tratadas em rega de espaços verdes, nomeadamente de campos de golfe, tem muito futuro em Portugal, como apoio ao turismo e à qualidade de vida dos portugueses. Portugal dispõe actualmente de uma significativa taxa de cobertura do país com serviço de tratamento de águas residuais urbanas, o que representa a produção de águas residuais tratadas ao nível de tratamento secundário e terciário de portuguesa. Estima-se que, sem recurso a armazenamento sazonal, o aproveitamento do efluente secundário das ETAR existentes em Portugal seria suficiente para cobrir pelo menos 10% das necessidades de água para rega. O efluente secundário pode ser utilizado na rega de campos de golfe, desde que seja objecto de tratamento complementar que reduza a quantidade de microrganismos de origem fecal a valores que assegurem que o contacto dos jogadores com a relva regada não origina problemas sanitários. Este é o caminho adoptado em muitas regiões, entre as quais a vizinha Espanha, e que começa a ser seguido em Portugal, liderado pelo Algarve, reconhecido como um dos melhores destinos de golfe do mundo.

MODELAÇÃO COM ELEMENTOS SÓLIDOS DE UMA CONSTRUÇÃO EM TERRA CRUA COM VÁRIOS TIPOS DE REFORÇO SUJEITA À ACÇÃO SÍSMICA

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Publicado em:
Jornal da Universidade do Minho - Engenharia Civil, 2008, 32, 43-56.

Neste artigo, baseado na dissertação de mestrado da primeira autora (Gomes, 2008) e dedicado à construção sismo-resistente em terra crua, após uma primeira descrição dos tipos de reforço utilizados nas várias estruturas modeladas, analisa-se o comportamento destas estruturas relativamente às tensões máximas obtidas e à sua admissibilidade. As estruturas apresentam as dimensões e características que podem ser consideradas representativas de um conjunto razoável de construções deste tipo, com dimensões em planta 13 x 14 m² e disposições construtivas dentro dos limites recomendados por especialistas em edificações em terra crua. Neste estudo recorreu-se à modelação informática de estruturas com elementos finitos tridimensionais, usando o programa de *software* para análise estrutural, SAP 2000 (*Structural Analysis Program*), versão 10.0.1..

MECHANICAL PERFORMANCE OF LAP JOINTS OF FLAT ROOF WATERPROOFING MEMBRANES

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This paper aims at portraying the influence of the type of membrane, the execution process of the lap joints, and their width on their mechanical performance, when subjected to forces that try to reproduce the stresses that lap joints undergo especially due to wind action. This effect on waterproofing membranes is treated in detail in the corresponding EOTA Guideline5 where the tests referred to later on also deserve some emphasis.
The research work reported here involved performing shear and peel resistance tests in three different membranes: atactic polypropylene (APP)-modified bituminous membrane, styrene-butadiene-styrene (SBS)-modified bituminous membrane, and thermoplastic polyolefins (TPO) membrane. For APP and SBS membranes, lap joints 50- and 100-mm wide made both with welding gas torch and hot air were tested. For TPO membrane, lap joints 20-and 40-mm wide made with hot air were tested. It must be referred that the shear and peel resistance tests are equally part of the harmonized European standards on the bituminous and synthetic membranes' characteristics that support their CE marking.

Publicado em:
Experimental Mechanics Journal, Jan/Fev 2008, 50-57.

O ATERRO SANITÁRIO COMO BIOREACTOR: DESAFIOS GEOTÉCNICOS

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Publicado em:
Revista Geotecnia nº 114, Nov 2008.

Em Portugal, no âmbito da gestão dos RSU e face à situação existente no ano de 1996, os aterros sanitários foram então encarados como a solução privilegiada para a resolução do passivo ambiental. Face à preocupação de contaminação dos solos e das águas subterrâneas, estes aterros foram projectados com um sistema de confinamento de fundo para isolar os resíduos do exterior, um sistema de cobertura para minimizar a entrada da água das chuvas e consequentemente a produção dos lixiviados, um sistema de drenagem, captação e tratamento de lixiviados e um sistema de drenagem, captação e tratamento de biogás.

Um outro tipo de abordagem, que ultimamente tem vindo a ganhar adeptos, recorre à técnica da recirculação dos lixiviados ou da injecção de outros líquidos, ou até de ar, na massa de resíduos depositados, em condições controladas, utilizando o aterro como um reactor biológico. Esta tecnologia implica uma mudança de perspectiva sobre o objectivo do aterro, que deixa de ser um mero depósito de resíduos para passar a ser também um local de tratamento de resíduos. Este artigo tem por objectivo, por um lado, mostrar as diferentes técnicas operacionais empregues e num aterro bio-reactor e as respectivas vantagens e desvantagens relativamente ao aterro dito "convencional". Pretende, também, chamar a atenção para os problemas geotécnicos que podem surgir com o emprego desta nova tecnologia e indicar algumas recomendações para os obviar.

AS TIC NO ENSINO DA GEOTECNIA: O ENSAIO VIRTUAL DE CORTE DIRECTO

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Tradicionalmente, recorre se à componente experimental no ensino da geotecnia para consolidar princípios e conceitos teóricos. No entanto, os alunos nem sempre estão preparados para apreciar o valor efectivo dessas experiências laboratoriais quer por não ser possível uma tutoria personalizada de acordo com as necessidades individuais, por causa do elevado número de alunos, quer devido a limitações de espaço, tempo ou número de equipamentos disponíveis. As dificuldades indicadas podem ser ultrapassadas com recurso a ensaios virtuais que permitam a simulação de experiências para diferentes condições iniciais, solicitações e tipos de materiais, conseguindo-se assim uma compreensão mais abrangente do comportamento dos solos. Neste contexto, iniciou-se a concepção de um ensaio virtual de corte directo, cujos objectivos, a estrutura da aplicação interactiva e os benefícios pedagógicos são apresentados neste artigo.

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AS VARIÁVEIS EXPLICATIVAS DO VALOR DE FRACÇÕES DE ESCRITÓRIOS

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O conceito avaliação imobiliária ou atribuição de valor a um bem imobiliário engloba uma complexidade de dados que nem sempre são tidos em conta no processo de uma avaliação concreta. Isto porque a actividade de avaliar engloba ramos do saber tão diversos como a engenharia civil, a econolia, o direito do urbanismo, a fiscalidade, a arquitectura, a engenharia mecânica, o urbanismo, a engenharia do território, as ciências sociais e humanas, etc. Como tal, e devido à escassez de bases de dados e de estudos de base nesta área, a atribuição de valor a um bem imobiliário é normalmente baseada na intuição e experiência do avaliador que a realiza.

De forma a tornar mais objectivo este processo, foi desenvolvido um trabalho de investigação no âmbito do segmento escritórios, do qual se apresenta neste artigo a parte inicial. Começa-se por expor o tratamento dos dados ou variáveis que mais directamente influem no valor de avaliação na óptica de mercado de uma fracção de escritório. Entendem-se como variáveis, as cinco vertentes segundo as quais devem ser analisadas as características de um imóvel, no que respeita à sua valorização: localização, equipamentos envolventes, características arquitectónicas, desempenho tecnológico, área. Cada uma destas variáveis é então discretizada por sub-variáveis e cada sub-variável por indicadores, os quais lhe atribuiem níveis de valor. O tratamento matemático estipulado para este estudo, fazendo o cruzamento entre as características do imóvel e o seu nível de importância, conduz à atribuição de um valor numérico único para cada fracção, denominado “Nível da Fracção”. O seu cálculo é aqui apresentado e exemplificado.

ACÇÕES SÍSMICAS EM ESTRUTURAS DE CONTENÇÃO

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As estruturas de contenção, normalmente sub-divididas em estruturas autoportantes (muros de gabiões, muros de betão armado funcionando como consolas verticais ou dotados de contrafortes, etc.) e estruturas ancoradas (paredes moldadas, paredes do tipo "Berlim Definitivo", cortinas de estacas-pranchas, etc.), devem ser dimensionadas para as acções sísmicas. Embora se possa pensar que a ocorrência dum sismo em simultâneo com a conclusão duma escavação geral a jusante duma cortina de parede moldada ancorada, possa ser pouco provável, a realidade mostra que, sempre que ocorre um sismo numa zona urbana nalguns locais desta existirão, certamente, escavações executadas ao abrigo de paredes moldadas que ainda aguardam a execução dos pisos enterrados para que a obra de contenção periférica se conclua.

Assim, faz todo o sentido admitir que se deve introduzir a acção sísmica no dimensionamento duma cortina de parede moldada como nos restantes tipos de estruturas de contenção.

Na presente comunicação é referida a forma de considerar a acção sísmica de acordo com as recomendações dos Eurocódigos estruturais, nomeadamente os EC7 e EC8.

Apresenta-se, ainda, um exemplo de aplicação a um caso de paredes moldadas ancoradas, já anteriormente dimensionado só para as acções estáticas [Matos e Silva, 2004], adoptando um método simplificado de dimensionamento de paredes moldadas publicado pelo autor [Matos e Silva, 2000].

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DEVELOPMENT OF AN IN SITU PENETRATION TEST FOR THE UPTAKE OF PRESERVATIVES IN APPLIED WOOD

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There are several buildings, in Portugal and particularly in Lisbon, with a three-dimensional triangular timber structure called gaiola (birds cage), which was imposed after the big earthquake of 1755 in order to guarantee the required seismic resistance of the buildings. The gaiola, composed of timber floors and timber-reinforced masonry load bearing walls, was meant to support vertical loads and to give lateral restrain to the exterior masonry walls, leading to a solid interaction between different structural materials and producing a strong, light and energy dissipative structure.

This structural design with its unique elasticity and anti-seismic characteristics, represents an important historical testimonial, namely of craftsmanship and engineering, making the preservation of such structures truly meaningful. In spite of this importance, and mainly after the expansion of the concrete use, maintenance on these buildings has become a rare event. Consequently, the late XXth century was marked by an overall poor condition of old buildings with an intense focus on the degradation of the wood components.

Biological degradation, in particular by the action of wood-rotting fungi, is the most common factor affecting wood structural elements in buildings. In order to maintain the highest number of original timber elements under maintenance or rehabilitation actions, in situ preservative treatments play an important role. However, in old buildings, the application of a curative/preventive measures is often impaired by the presence of previous treatments or finishes not always well documented and difficult to characterize.

Within the development of a PhD project concerning the rehabilitation of degraded timber structural elements due to biological agents, through laboratory and in situ analysis, the need arise to develop a penetration test that would allow a swift evaluation of the possibility to re-treat with a certain new wood preservative with minimum disturbance to the structure under rehabilitation.

Three types of products were considered as representative of previous treatments of old structures, namely, oil-borne preservatives (e.g. pentachlorophenol or creosote), light organic solvent preserva-

tive (LOSP) using white spirit as the solvent carrier to deliver the actives into timber and arsenic copper combinations such as chromated copper arsenate (CCA). The later was not considered relevant under the present study.
This paper describes the test developed and presents the results of its calibration for untreated maritime pine (Pinus pinaster Ait.) and for maritime pine treated with either an oil carrier formulation or a typical LOSP formulation.
Two newer, more environmentally benign products were chosen for the re-treatment, one water borne product (boron based) and a water dispersible organic formulation. Their ability to penetrate the pre-treated surfaces was evaluated after 1, 2 and 3 applications at 24 hours intervals and the results obtained are presented.
Finally, the applicability of the developed test to the in-situ evaluation of timber structures is also discussed.

DIAGNOSIS OF OLD TIMBER STRUCTURES. THE CASE OF THE FUTURE WINE MUSEUM OF BUCELAS

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The need to intervene in timber structures is very frequent and especially so in the rehabilitation or conservation of ancient buildings, due not only to its frequent presence as a structural material but also to its susceptibility to various degradation agents, such as fire, several physical, chemical, mechanical and mostly biological agents, the latter being the most common and those that imperceptibly lead to most grievous damage. Notwithstanding its susceptibility, timber is a material endowed with high structural characteristics and with excellent durability when adequately selected, treated, applied and maintained. Interventions in timber structures must be defined after a thorough evaluation of its conservation state, always having as a first objective the achievement of its recovery and/or maintenance. Therefore, this paper will present the diagnosis work that must be performed to evaluate the conservation state of a roof structure in which the four most common degradation agents in Portugal were simultaneously detected: wood rot, termites, Hylotrupes bajulus and Anobium punctatum. The building used as a case study, the future "Wine Museum of Bucelas", dated from 1887, underwent in the latest years a total lack of maintenance, the main reason why all these biological degradation agents had every condition to increasingly install themselves. The inspection work performed and the results obtained will be presented not only descriptively but also graphically. The design and maintenance deficiencies of the building roof that led to the present damage level will also be presented and related to the degradation problems they cause. The level of the damage detected will also be analyzed.

NORTH EAST ATLANTIC TSUNAMIS: UPDATE OF THE PORTUGUESE CATALOGUE OF TSUNAMIS

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Catastrophic tsunamis are described in historical sources for all regions around the Gulf of Cadiz, at least since 60 BC. Most of the known events are associated with moderate to large earthquakes and among them the better studied is the 1st November 1755. We present here a review of the events which effects, on the coasts of the Portuguese mainland and Madeira Island, which are well described in historical documents or have been measured by tide gauges since the installation of these instruments. For a few we include new relevant information for the assessment of the tsunami generation or effects, and we discard events that are included in existing compilations but are not supported by quality historical sources or instrumental records. We quote the most relevant quantitative descriptions of tsunami effects on the Portuguese coast, including in all pertinent cases a critical review of the coeval sources, to establish a homogenous event list. When available, instrumental information is presented. We complement all this information with a summary of the conclusions established by paleo-tsunami research. This research was funded by NEAREST and TRANSFER, 6FP EU Projects.

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IMPLEMENTATION OF THE NEAMTWS IN PORTUGAL

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After the tsunami of December 2004, the UNESCO, through its International Oceanographic Commission, recognized the need for an end to end global tsunami warning system and International Coordination Groups have been established for different areas around the globe: Indian, Caribbean, Atlantic and Mediterranean ocean basins. This system is the natural response to the historical and recent instrumental events generated along the western segment of the Eurasia and Nubian plates, which eastern end corresponds to the Gulf of Cadiz. The TWS includes three main components: the seismic detection, the tsunami detection and the issue of warnings/alerts. In Portugal the automatic earthquake processing is installed at IM (Instituto de Meteorologia) which is the only national institution operating on a 24x7 basis. This makes IM the natural candidate to host the Portuguese tsunami warning system. The TWS under implementation has several key points: definition of the tsunami scenarios, tsunami detection, and tsunami protocol messages. The system will also be able to predict tsunami potential impact along the coast, wave-heights and arrival times at pre-defined locations along the coast. In this study we present the recent results on definition of tsunami scenarios, establishment of the scenario database and the tsunami analysis tool. This work is a joint effort between Instituto de Meteorologia (Portugal), the Joint Research Center, JRC- ISPRA, Italy and the coordination of the Portuguese Group for the implementation of NEAMTWS in the area. This work has been financed by different European projects as NEAREST and TRANSFER, and also by the JRC, the IM and CGUL/IDL institutions.

INUNDATION PATTERNS IN HUELVA, SW EUROPE, DUE TO TSUNAMI IMPACT

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This study describes the activity conducted, in the framework of TRANSFER EU, STREP37058, on the test area of Huelva, Spain. This is, un-doubtfully, one of the most affected areas in case of a tsunami event generated in the Gulf of Cadiz (SW IBERIA). Historical records and sedimentary deposits suggest that the area has been hit by several tsunamis during the Holocene. The Huelva estuary is formed by the confluence of the rivers Tinto and Odiel. This is an interesting case study due to the fact that the area is characterized by vary shallow topography, making it prone to tsunami inundation; the fact that the estuary is an alternate pattern of dry and wet areas makes the interpretation less straightforward than in areas with a simpler geometry. Inundation studies are performed using model earthquake, of magnitude 8.1 – 8.75, representing the “typical faults” in the Gulf of Cadiz area. The tsunami generation is simulated assuming that the initial wave profile follows the deformation of the ocean and that this deformation can be calculated using the Okada's equations. A sensitivity analysis due to variations in source parameters, dip and strike angles and slip along the fault plane is addressed. Each source parameter study is allow to vary separately in order to isolate its influence in run up and flow depth at the coast. The results are presented in terms of flow depth maps.

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LONG TERM HAZARD FROM ATLANTIC SUBDUCTION ZONES (ANTILLES AND CADIZ/GIBRALTAR) AND THE EXAMPLE OF THE GREAT LISBON EARTHQUAKE AND TSUNAMI OF 1755

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While great earthquakes and associated tsunami occur far less frequently in the Atlantic than in the Pacific, such events have occurred in the past. The two most recent destructive events were the 1929 Grand Banks earthquake and tsunami and the Great Lisbon earthquake and tsunami of 1755. The main cause for this discrepancy (beyond the smaller size of the ocean basin) is the abundance of subduction zones in the circum Pacific region and the near absence of such tectonically active zones in the Atlantic. Nevertheless, there are slowly converging subduction zones in the Atlantic, the Antilles arc (which has not produced any great earthquakes in the past 150 years and the Gibraltar/Gulf of Cadiz arc (offshore SW Iberia, whose activity remains controversial). We present new research on these two zones. In both cases, deep seismic sounding data together with earthquake hypocenters are used to construct lithospheric cross-sections. These form the basis for thermal modeling in order to determine the probable dimensions (downdip width) of the potential seismogenic fault plane. Tsunami modeling has been performed for the Cadiz/Gibraltar subduction zone using these calculated limits and wave propagation models have been established. These predict the regional impact (travel-times and amplitudes) as well as the far-field effects of a subduction fault plane source for the 1755 tsunami. Indeed, this event produced a 5-10 m tsunami on the S. Portuguese, SW Spanish and NW Moroccan coasts. It was also observed (1-5 m waves) in the Antilles. Work on the Antilles subduction zone has only recently begun. Here strong events last struck in 1839 (intensity IX in Martinique) and 1843 (intensity X in Guadeloupe). Thermal modeling suggests the seismogenic zone is widest to the south, where the accretionary wedge is widest. This region is marked by a total absence of instrumentally recorded thrust type earthquakes (just as is the entire Gulf of Cadiz). Comparative analysis of subduction zones worldwide suggests that those with the slowest convergence rate typically have the longest recurrence intervals and thus, behavior over the past 100 years may not offer a reliable estimate of long-term hazard. More detailed studies will be necessary in order to properly assess the natural hazard posed by this region (over 1000 km in length), such as better information on the crustal structure.

TSUNAMIGENIC SOURCE AREAS FOR PORTUGAL MAINLAND, IBERIA

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Tsunami hazard and risk assessment is presently a powerful tool for decision planners and land users authorities. After the Boxing day catastrophe the civil authorities of most European countries, affected by tsunamis in the past, are most aware of the importance of evaluation of tsunami impacts. The goal of this study is to present a summary of the knowledge gathered by the scientific Portuguese community in what concerns the identification of active tectonic structures that can trigger alone or in a specific combination, a mega-tsunami similar to those that are known to stroke the Portuguese coasts in the past. It is far beyond the scope of this study the support/not of any new or old interpretation of a specific seismic event.

A coarse segmentation of the potential tsunamigenic source zone (SZ), defining for each one the Maximum Credible Earthquake (MCE) and associated Typical Fault (TF) is presented. We will allow the TF to "float" along the SZ at regular intervals to produce a set of tsunami scenarios that can be described as the Worst Case for the Portuguese coast. This zonation allows for the computation of inundation maps and a set of hydrodynamic parameters for all target areas. This study is a joint effort of tasks WP 1 Tsunami source identification of NEAREST project, WP2 – Tsunamigenic seismic sources of TRANFER project and constitutes a valuable tool for seismic and tsunamigenic risk evaluation of the Algarve area. The work presented here was funded by ERSTA - ANPC (Portuguese Civil Protection); TRANSFER Project 6FP contract 37058 And NEAREST Project 6FP contract 37110.

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TSUNAMI DETECTION NETWORK FOR THE GULF OF CADIZ

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Gen. Ass. European Seismological Commission, Crete, Greece.

After the Boxing Day tsunami 2004, the world increased awareness of the threat posed by tsunamis. In early 2005 the IOC-UNESCO decided to implement a global tsunami warning system, including four main regions: Indian Ocean, Pacific Ocean, Caribbean and North East Atlantic, Mediterranean and connected seas (NEAM).

The eastern end of the Nubia-Eurasia plate boundary, close to the Gulf of Cadiz, has been the place of several tsunamis, like the well known event of November 1755. During the 20th century several tsunamis were recorded in the area: 25 November 1941, 28 February 1969. The extensive occupation of coastal areas in the surrounding countries – Portugal, Spain and Morocco and the enormous influxes of tourists during high season increases the risk of tsunami impact.

In August 2007 an abyssal observatory was deployed 150 km SW of, Portugal. The choice for the location of the station was based upon the present understanding of seismogenic/tsunamigenic structures in the area.

PODEMOS PREVER UM TSUNAMI?

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O tsunami gerado pelo sismo de 1 de Novembro de 1755 foi o maior desastre natural verificado em Portugal. O sismo ocorreu cerca das 9h30, hora de Lisboa, tendo sido sentido um pouco por toda a Europa. O tsunami foi observado no Atlântico Norte, desde as Ilhas Barbados até à Escócia; no entanto as ondas mais destrutivas ocorreram em Portugal Continental, Espanha (Golfo de Cádiz) e no Norte de Marrocos. As dimensões catastróficas deste evento deram origem a uma onda de solidariedade e de consternação a nível global. Passados cerca de duzentos e cinquenta anos, no início do século XXI, a Humanidade assiste quase em directo, pela televisão, ao desenrolar de duas catástrofes naturais de grandes dimensões: o tsunami de Sumatra e o furacão Katrina. O que tiveram em comum estas duas catástrofes? Ambas são fenómenos altamente energéticos e com um elevado poder devastador; por outro lado, verificou-se a incapacidade de ser prestado auxílio às populações em fuga e a enorme vulnerabilidade dos locais atingidos, quer se trate de um dos países mais ricos do mundo ou do litoral mais pobre do oceano Índico. Os tsunamis têm um potencial destrutivo enorme, sendo gerados por grandes sismos, por gigantescos deslizamentos de terrenos ou por grandes explosões vulcânicas. Os furacões são gerados pela evolução de tempestades tropicais, em regiões onde a temperatura da água do mar à superfície é elevada. Se bem que envolvendo escalas temporais distintas, ambos são fenómenos globais no que diz respeito ao impacto social e económico. Quatro anos passados sobre o grande tsunami de Sumatra em que ponto nos encontramos? Quais os avanços científicos nesta área? Qual a resposta dos países e das organizações mundiais a futuros fenómenos semelhantes a um grande tsunami? O que foi feito em Portugal? Às 22h14 do dia 25 de Agosto de 2007 foi colocado o primeiro observatório submarino integrado na rede de alerta precoce de tsunamis em instalação no Golfo de Cádiz. Este acontecimento é parte de um conjunto de projectos que visa dotar as populações da área do Golfo de Cádiz de um sistema integrado de alerta precoce.

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SEGURANÇA DAS CONSTRUÇÕES EM TERRA CRUA FACE À ACÇÃO SÍSMICA

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A utilização da terra tem servido não só para a construção de habitações rurais e urbanas mas também para erguer grandes monumentos. Este tipo de construção surgiu como resposta à grande carência habitacional em algumas zonas do globo e esta está directamente relacionada com a escassez de recursos financeiros das populações dessas mesmas zonas, sendo de grande importância a revitalização do uso da terra como material de construção em diversas zonas. As tecnologias tradicionais de construção com terra são variadas, com inúmeras adaptações à qualidade da mesma, à identidade das culturas e aos lugares, de acordo com as diferentes experiências e com as formas de pensar da sociedade e da época onde se integram.

A terra será sempre um dos materiais contemplados na construção das habitações, em particular nas regiões economicamente mais carenciadas, devido à sua abundância, custo acessível, tradição (em alguns países) e facilidade de execução. No entanto, os problemas energéticos, ambientais, ecológicos e económicos sentidos a nível mundial conduzem a uma mudança de mentalidades nos escalões privilegiados das sociedades desenvolvidas. A terra crua como material de construção deixou de ser sinónimo de desconforto e pobreza para começar a ser vista como um material alternativo e valorizado. Como tal, por todos os continentes, está actualmente em curso um revivalismo da arquitectura de terra.

As principais causas de degradação deste tipo de construção são: degradação física ao longo do tempo, principalmente devido à acção da água e chuvas; e fraca resistência mecânica do material, quando solicitado aos vários tipos de acções, nomeadamente a acção sísmica. Face ao exposto, questionou-se como simular correctamente o comportamento dos materiais utilizados nas construções de terra e qual o método mais adequado para averiguar a sua segurança face às acções sísmicas.

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

POPULATIONAL GROWTH MODELS IN THE LIGHT OF SYMBOLIC DYNAMICS

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Understanding the structural aspects of the dynamic of populations, so that we can forecast their future evolution, is an important decision tool in demographic and economic planning, essential for management in many branches of Biology, such as the preservation of the environment, wildlife management, restrictions in fisheries, or pests control.

Sophisticated random models are now available in population dynamics, but in many instances their mean functions are well known deterministic models, useful as a first approach in applied problems. The logistic Verhulst (1845) model, which incorporates in its parameters both the mendelian growth rate and the retroaction due to the limitation of natural resources, is a natural candidate to model the dynamic of non-overlaping generations, namely when the unit of time is related to the life span of the individuals in the population. More general stochastic models (birth and death, branching) and the deterministic counterparts given by their mean functions are useful in more complex situations.

An interesting point of the Verhults model is its usefulness in dealing with the extinction of species. In fact we know that a large percentage of species became extinct, even when their reproduction rate seemed to be quite successful. The theory of dynamical systems applied to the Verhulst model in fact predicts the extinction of species with high reproduction rate, and population dynamics now interprets this as a side effect of over-success triggering the over-success of the species enemies (predators, viruses, diseases caused by microorganisms, etc.); the co-integration of the series of rabbit and fox furs caught at Hudson Bay, Canada, over the years shows that ultimately both species can become extinct as soon as the natural re-equilibrium fails. In this perspective, the fractal and chaotic behaviors of the population size N(t) when the mendelian reproduction rate is high is a strong point in favor of using a dynamical systems approach in modeling life phenomena.

The Verhults model can be easily presented as an approximation granted by the Taylor series expansion. If the population size N(t) is

a regular function such that $\frac{d}{dt}N(t) = A_o + A_1N(t) + A_2N(t)^2 + \ldots$, truncating the terms of order greater than 2, $\frac{d}{dt}N(t) = A_1N(t) + A_2N(t)^2$, with A1 › 0, and A2 ‹ 0. In fact, A0 must be 0, since an extinct population cannot produce progeny, A1 › 0 because while resources are abundant the population has a tendency to grow, and A2 ‹ 0 is a retroaction feedback due to scarce natural resources due to the population growth. This equation can thus be written $\frac{d}{dt}N(t) = rN(t)\left(1 - \frac{N(t)}{k}\right)$ the classical expression of the Verhults model.

But on the other hand, for non-overlaping generations populations we can use a discrete approach, replace this differential equation by the difference equation $x_{n+1} = r\, x_n\, (1 - x_n)$, with n = 0,1,2,...

whose right-hand side is proportional to the beta density, with both shape parameters equal to two, which is denoted by Beta(2,2) density. The numerical study, using the fixed point method, of the limit behaviour of this "logistic parabola", is at the core of spectacular developments in dynamical systems. The rationale of truncation terms of higher order in the Taylor series expansion, as done in developing the Verhults model, is simplicity, as expressed in Occam's razor metaphor, but also the prejudice that in non-overlaping generation populations the life-span of its members is one unit.

In this paper we investigate, along similar lines, the fractal and chaotic behaviour of models proportional to other Beta(p,2) densities, plausible when the reproduction paradigm of the population is more general.

FAMÍLIA PARAMETRIZADA GLE

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Para facilitar o trabalho de investigadores que pretendam usar uma família que contém como casos especiais a Gaussiana e a Laplace (caso simétrico) e a Gaussiana dobrada e a Laplace dobrada (no caso de suporte em $(0,\infty)$), discutimos como gerar números pseudo-aleatórios com essa distribuição Gaussiana-Laplace Estendida (GLE), e publicámos electronicamente, em www.ceaul.fc.ul.pt, listagens de pseudo-aleatórios GLE, para valores adequados do parâmetro de forma.
A nossa motivação inicial foi investigar o papel da rarefação de Rényi em amostragens com taxas elevadas de não resposta, e robustez de estimadores de localização e escala em populações não gaussianas.
Considere-se a família de variáveis aleatórias W_β com funções densidade de probabilidade

$$f_{W\beta}(x) = \frac{\exp(-x)^\beta}{\Gamma\left(1+\frac{1}{\beta}\right)} I_{(0,\infty)}(x),$$

Adiante estabelecemos relações simples W_β com produtos de potências de gamas independentes, que usamos para a geração de números pseudo-aleatórios daquelas populações.
Começamos por descrever as propriedades estruturais importantes, e os métodos usados para geração dos números pseudo-aleatórios dessa família. Descrevemos ainda os métodos usados para avaliar se os números pseudo-aleatórios assim gerados se ajustam convenientemente às leis que pretendemos usar.
O mesmo fazemos com uma família de variáveis aleatórias simétricas X_{β^*}, que inclui a Gaussiana e a Laplace, e que se obtém de forma simples multiplicando uma variável aleatória positiva da classe anteriormente descrita por uma Bernoulli simétrica independente. Por uma questão de conveniência, optamos por uma parametrização em que o parâmetro de forma é $\beta^*=(2-\beta)/\beta > -1$:

$$f_{x\beta^*}(x \mid \beta^*, \lambda, \delta) = \frac{1}{2^{\frac{\beta^*+3}{2}}\,\Gamma\left(\frac{\beta^*+3}{2}\right)\delta} \exp\left\{-\frac{1}{2}\left|\frac{x-\lambda}{\delta}\right|^{\frac{2}{1+\beta^*}}\right\} I_{\mathbb{R}}(x),$$

A família $\{W_\beta\}_{\beta>0}$ é referida como família GLE com suporte positivo; e a família $\{X_{\beta^*}\}_{\beta^*>-1}$ como família GLE com suporte real.

01

THE CHARACTER AND PROPAGATION OF MIOCENE COMPRESSION IN THE TAGUS ABYSSAL PLAIN

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8º Conferência Anual do GGET, 24-25 Julho, Memórias do Dep. Geologia, Univ. Porto, Porto, 2008, nº13, pp. 99-102.

The effects of the Miocene through Present compression in the Tagus Abyssal Plain are mapped using multi-channel seismic reflection and refraction data. Four distinct structural domains are recognized along seismic line IAM5. The Miocene tectonic inversion is mainly accommodated in Domain 3 by oceanwards directed thrusting at the ocean-continent transition and continentwards on the continental slope. Rheological numerical modelling indicates that the frictional strength in the ocean-continent transition zone is reduced in 30% relative to the surrounding regions.

ASPECTOS METODOLÓGICOS NA ANÁLISE MULTIVARIADA DE "CLUSTERS" SOCIOECONÓMICOS DE BASE REGIONAL

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Este artigo sintetiza os diferentes aspectos metodológicos relacionados com a estimação multivariada de "clusters" socioeconómicos de base regional, enunciando diversos casos de aplicação presentes na literatura dos últimos anos. É discutido o problema da escolha das variáveis, da necessidade de redução de dados, e da escolha do método de classificação/agrupamento. É usado um caso de estudo envolvendo indicadores socioeconómicos da base de dados Régio do Eurostat para comparar a variabilidade dos resultados causada pela selecção das variáveis com a resultante da escolha de diferentes métodos de classificação/agrupamento.

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COMPARISON OF SEISMIC REINFORCEMENT SYSTEMS IN A SMALL BUILDING WITH MASONRY WALLS

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In this paper it is presented a comparative analysis of the application of several solutions of seismic reinforcement in a small building, with two floors, built with masonry walls and wood pavements.
The first phase of the study consists of the numerical modelling of the referred building with a f.e.m. program (SAP2000®), where a dynamic analysis was accomplished, assuming that the whole structure would have a linear elastic behaviour.
In a second phase, it was considered the simulation of the application of several solutions of seismic reinforcement to the original model of the building, namely:

1. Steel beams placed in the external walls, at the level of the pavements;
2. Layer of reinforced mortar applied in one of the faces of the walls;
3. Layer of reinforced mortar applied in both faces of the walls;
4. Layer of composite material (glass fiber reinforcement) applied on the two faces of the walls;
5. Layer of composite material (carbon fiber reinforcement) applied on the two faces of the walls;
6. Crowning concrete beam placed in the top of the walls;
7. External steel cables, placed at the level of the pavements;
8. New structure (concrete columns and steel beams) embedded in the stone wall;
9. Steel H beams placed over doors and windows;
10. Steel H frames placed in doors and windows.

Finally, the third phase consists in the comparative analysis of the results, before and after reinforcement, considering the frequency values, displacements in the top of the walls, displacements in the top of doors and windows and the value of the tensile stresses in the masonry.

ANÁLISE DE CUSTOS EM OBRAS DE REABILITAÇÃO DE EDIFÍCIOS

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A presente comunicação apresenta o trabalho que está a ser realizado sobre a análise de custos em obras de reabilitação de edifícios no Laboratório Nacional de Engenharia Civil (LNEC), no âmbito do projecto PRONIC (Protocolo para a Normalização da Informação Técnica da Construção).
As obras de reabilitação de edifícios são realizadas cada vez em maior número e a necessidade da quantificação económica, de uma forma sistemática e organizada, dos trabalhos de intervenção em edifícios existentes, já se faz sentir. Assim, a oportunidade de fazer uma recolha exaustiva de custos de trabalhos de reabilitação e reforço de edifícios surgiu com o projecto PRONIC. Este projecto, que está a ser desenvolvido por um consórcio formado pelo Instituto da Construção (IC) na FEUP, pelo LNEC em Lisboa e pelo INESC no Porto, é constituído por uma aplicação informática onde foram definidos trabalhos de construção numa estrutura de capítulos, existindo um articulado com vários níveis dentro de cada capítulo. Os trabalhos de construção são arrumados nesta estrutura, constituindo o seu nível inferior, sendo necessário definir para cada um deles uma ficha técnica de material, uma ficha de execução de trabalho e uma ficha de composição de custo. O PRONIC fornece uma base de informação que contempla, para além dos trabalhos correntes em obra nova, trabalhos específicos realizados em obras de reabilitação e de reforço.
Desta forma, com base nas descrições dos trabalhos de reabilitação de edifícios existentes no PRONIC e com a colaboração das empresas de construção e entidades promotoras deste tipo de intervenções em edifícios existentes, estão a ser levantados os custos unitários desses trabalhos e a respectiva composição de recursos. Os custos unitários das tarefas neste tipo de obras são difíceis de quantificar, pois baseiam-se ainda muito na experiência e observação global de trabalhos. Como em Portugal, este tipo de intervenções é relativamente recente, ainda não houve tempo para se proceder à recolha e uniformização desses valores, que se tornam cada vez mais urgentes e necessários na preparação de novos projectos. No entanto, existem já algumas bases de dados sobre obras de reabilitação noutros países da Europa, tais como na Espanha, na Itália e na Inglaterra. Na continuidade deste trabalho que está a ser realizado, vai ser feita uma análise de custo/benefício sobre a introdução de reforços estruturais (melhoria do comportamento do edifício sob a acção de um sismo) em obras de reabilitação.

UTILIZAÇÃO DE BETÃO AUTO-COMPACTÁVEL (BAC) - UMA ANÁLISE DE VIABILIDADE ECONÓMICA

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Publicado em:
Actas do Encontro Nacional de Betão Estrutural 2008, Guimarães, 5, 6 e 7 de Novembro de 2008, pp. 287-288.

O presente artigo tem como objectivo levar a cabo uma análise económica da utilização de betão auto-compactável (BAC) na construção de edifícios e que vá um pouco mais além da "simples" quantificação dos custos directos relativos tanto à matéria-prima e produção como à quantificação de mão-de-obra a associar à tarefa específica de colocação em obra de BAC.
Desse modo, para além do referido, será feita uma análise comparativa entre BAC's produzidos utilizando dois métodos de cálculo de amassaduras propostos por dois investigadores nacionais em trabalhos anteriores e betões convencionais de comportamento considerado equivalente. Serão igualmente abordados os benefícios indirectos da utilização do BAC, que são claramente mais difíceis de traduzir em termos económicos quando comparados com os benefícios directos. Por outras palavras, entende-se no presente trabalho que a utilização de BAC na indústria da construção civil não tem exclusivamente impacte nos referidos custos directos mas tê-lo-á também a outros níveis e de um modo não menos importante.

EDIFÍCIO EM LISBOA: ESCAVAÇÃO E CONTENÇÃO PERIFÉRICA, PLANO DE INSTRUMENTAÇÃO

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Neste artigo são enumerados os principais critérios de concepção e de execução adoptados nas soluções de escavação e contenção periférica de um edifício construido no centro de Lisboa, contíguo ao edifício do Serviço de Estrangeiros e Fronteiras. A escavação necessária à construção do referido edifício apresenta uma profundidade máxima de cerca de 28 m, intersectando aterros, formações Miocénicas e Neocretácicas. Face às características da envolvente, foi necessário garantir a manutenção de níveis de deformação reduzidos na estrutura de contenção e solo suportado, tomando particular importância o plano de instrumentação e observação implementado bem como os estudos e modelação numérica desenvolvidos, com o objectivo de aferir da compatibilidade entre a solução projectada e o comportamento real observado.

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REABILITAÇÃO ESTRUTURAL COM RECURSO À MICROESTACAS

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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 1,5m 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 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.
O facto das fundações das nascenças dos arcos assentarem mais do que as das paredes de empena, decorre duma maior concentração de cargas pontuais na base dos arcos em contraponto com cargas menores e mais distribuídas ao nível das fundações das empenas. Também o contacto com as fundações das empenas dos edifícios vizinhos favorece uma diminuição dos assentamentos das fundações das empenas em relação aos das nascenças dos arcos, originando o fenómeno que provocou as patologias detectadas.
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 127mm (5”). Nas nascenças interiores executaram-se duas microestacas de capacidade unitária 1000kN e diâmetro nominal de 152mm (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 10^3 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.

ACÇÕES SÍSMICAS EM PAREDES MOLDADAS

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Embora se possa pensar que a ocorrência dum sismo em simultâneo com a conclusão duma escavação geral a jusante duma cortina de parede moldada ancorada, possa ser pouco provável, a realidade mostra que, sempre que ocorre um sismo numa zona urbana nalguns locais desta existirão, certamente, escavações executadas ao abrigo de paredes moldadas que ainda aguardam a execução dos pisos enterrados para que a obra de contenção periférica se conclua.
Assim, faz todo o sentido admitir que se deve introduzir a acção sísmica no dimensionamento duma cortina de parede moldada.
Na presente comunicação é referida a forma de considerar a acção sísmica na aplicação do método simplificado de dimensionamento de paredes moldadas já anteriormente publicado pelo autor.
Apresenta-se, ainda, um exemplo de aplicação a um caso já anteriormente dimensionado, só para as acções estáticas.
De acordo com o Eurocódigo 8 – Parte 5 (pr EN 1998-5) as acções dinâmicas actuando sobre estruturas de contenção de terras devem ser quantificadas de acordo com o método de Mononobe-Okabe, o qual conduz a boas aproximações com a realidade.
Do parágrafo 7.3.2.2. do referido Eurocódigo, o coeficiente sísmico horizontal será:

$$k_h = a_{gr} \times \gamma i \times \frac{S}{g \times r}$$

(1)

em que, para cortinas ancoradas, dada a sua relativa flexibilidade, se considera r = 1,0.
Os restantes parâmetros da equação (1) são fornecidos pela norma portuguesa ENV 1988-1-1 e, para a acção sísmica do tipo 1 em zona sísmica A, tem-se:

$a_{gr} = 2{,}7$ $\gamma i = 1{,}0$ $S = 1{,}0$ $g = 10{,}0 m/s^2$

donde:

$$k_h = 0{,}27$$

Para solos coesivos é importante saber como pode variar o valor da coesão quando ocorre um sismo. De acordo com resultados experimentais a coesão diminui quando ocorre um sismo, considerando-se, habitualmente, que o valor da coesão sob as acções dinâmicas é da ordem de 80% do valor sob acções estáticas, o que é justificado por se presumir que as ligações de coesão entre as partículas de argilas e siltes possuem uma certa elasticidade possibilitando ligeiros deslocamentos oscilatórios repetidos dessas partículas, umas em relação às outras, sem que haja rotura das ligações. Esta prática está reflectida no parágrafo 3.1 do Eurocódigo 8, onde se recomenda, quando se considera a acção sísmica, a adopção de coeficientes de minoração para a coesão de 1,3 para cu e de 1,2 para c o que equivale a considerar cerca de 80% do seu valor sob as acções estáticas. Para além da acção dinãmica do solo sobre a cortina é necessário considerar a acção sísmica sobre a massa da cortina, que é dada por:

$$q' = k_h \times P \qquad (2)$$

em que:

k_h – coeficiente sísmico horizontal quantificado a partir da equação (1)

P – Peso próprio da cortina /m^2

É importante notar que o ponto de aplicação das acções estáticas + dinâmicas do solo sobre a cortina, no caso das estruturas de contenção rígidas, deve situar-se a meia altura dessas estruturas. Contudo, para cortinas flexíveis com possibilidade de rotação na sua base, o que acontece frequentemente nas cortinas de paredes moldadas (a menos que tenham uma ficha de comprimento excessivo), o EC8, no seu parágrafo 7.3.2.3, alínea 5), recomenda que se utilize o mesmo ponto de aplicação da resultante das acções estáticas. No que se refere à acção sísmica sobre a massa da cortina esta terá uma resultante que se encontra localizada a meia altura da cortina.

Da presente comunicação pode concluir-se que, numa cortina de parede moldada ancorada de grande altura, a acção sísmica é fortemente condicionante do seu dimensionamento.

Embora, como atrás dissémos, a probabilidade de ocorrência dum sismo, durante a fase de escavação geral ao abrigo duma cortina ancorada, seja pequena, dado o curto período de tempo em que essa escavação decorre, é imperativo que factores exógenos não prolonguem demasiadamente esse período de modo a que a probabilidade de ocorrência dum sismo aumente.

BEHAVIOUR MONITORIZATION OF A 13 M HIGH GABIONS WALL

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Apresentado na:
"Sixth International Conference on Case Histories in Geotechnical Engineering", Arlington, Virginia, EUA, Agosto de 2008.

The paper refers a gabions retaining wall, located at Belas, about 30 km West of Lisbon, in the North perimeter of an Organic Valorisation Central (Valorsul). After the wall completion some pathology occurred and it was detected that it had been partially executed with marl limestone blocks that loose mechanical resistance under rainy water. The wall was then demolished and rebuilt with adequate material. During the earth fill execution the wall was monitorized with a superficial topographical survey. The results obtained and the respective conclusions are referred.

CONSTRUÇÃO SISMO-RESISTENTE EM TERRA CRUA

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Universidade Técnica de Lisboa - Instituto Superior Técnico, 2008.

Sabe-se à partida que, em regiões sísmicas, as estruturas deverão ser projectadas e construídas de forma a limitarem os seus danos e principalmente a resistir às acções sísmicas sem pôr em causa a integridade dos seus utentes.
Pretendeu-se, com este trabalho apresentar um estudo sobre o comportamento sísmico de uma construção em taipa, visto que a vulnerabilidade sísmica deste tipo de estruturas é um problema muito relevante. Sabendo que voltaram a surgir em Portugal construções com terra crua, é necessário definir um conjunto de recomendações para a concepção em segurança das mesmas em zonas sísmicas (recorde-se que todo o território nacional o é), quanto ao melhor método construtivo e às melhores técnicas construtivas para uma construção 'sismo-resistente' com terra crua já que, em Portugal, não existe qualquer norma para a construção neste material estrutural.
Assim, optou-se por conceber um edifício com a tipologia corrente, de acordo com autores da área, com apenas um piso, servindo de base às cinco modelações. Cada modelação caracteriza uma estrutura com diferentes metodologias para fazer face à acção sísmica. Para a realização da análise dinâmica tridimensional, utilizou-se um programa de cálculo automático de estruturas SAP2000 *(Strutural Analysis Program)*, no qual se modelou o edifício. Este estudo foi fundamental para perceber qual o efeito da acção sísmica nas cinco modelações e qual o comportamento sísmico nestas construções.
A acção sísmica é considerada por intermédio de espectros de resposta definidos no Regulamento de Segurança e Acções e as propriedades do material terra são determinadas de acordo com alguns regulamentos internacionais e de acordo com as recomendações de autores desta área, novamente pela ausência de qualquer norma nacional para a construção em terra.
Identificam-se os principais esforços que actuam nestas estruturas e faz-se a verificação aos estados limite últimos nos modelos numéricos para cada uma das análises.
Por fim, são apresentadas conclusões acerca de todo o estudo, sugerindo-se ainda alguns desenvolvimentos futuros.

TEMAS EM MÉTODOS QUANTITATIVOS -PERSPECTIVAS DO CRÉDITO À HABITAÇÃO

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A actividade de atribuição de valor a um bem imobiliário apela e exige uma fundamentação teorico-prática consistente. Teórica, porque tem que se basear em critérios e princípios objectivos, derivados de formulações de base científica e amplamente aceites. Prática, porque emana de um exaustivo trabalho de campo que tem que ser sucessivamente reiniciado e repetido por cada novo imóvel que se pretenda avaliar. Se a parte teórica é de simples compreensão e de fácil execução, já a parte prática requer esforço físico, persistência e experiência, a qual só será adquirida... fazendo!
O presente texto pretende fornecer ferramentas teóricas de iniciação. Não descura contudo, a parte de trabalho de campo, chamando a atenção repetidamente para as mais diversas situações para as quais o avaliador deve estar atento. Inicia com a apresentação dos pressupostos que envolvem a actividade de avaliação imobiliária, descrevendo depois de uma forma sumária os métodos existentes e as suas especificidades, apresentando, por fim, uma forma de cálculo do valor de avaliação de uma fracção habitacional.

A COMPARED ANALYSIS OF THE PORTUGUESE REAL ESTATE INVESTMENT MARKET ON MATURITY AND TRANSPARENCY ISSUES

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Doutoramento em: Engenharia Civil
Grau Concedido por: Universidade do Minho
Orientadores: José Manuel Cardoso Teixeira e Elísio Fernando Moreira Brandão
Provas Concluídas em: 3 de Outubro de 2008

Most important theoretical developments in finance and investment have been put to widespread practical use, especially in the more efficient securities markets. Real estate investment research has followed these developments, with a 20 year lag, but to some extent, common practice of asset allocation in a property portfolio still relies on qualitative and subjective personal judgment. In Portugal, academic research on property finance is, at least, incipient.

The general objective of this research is the development of a compared analysis of the Portuguese real estate investment market in terms of its maturity and transparency, in order to evaluate the potential of attracting international investment and to provide with foundations for future development. Three fundamental issues are addressed: availability of quality information to develop consistent analysis to support managerial decisions, the existence and nature of institutional property investment and the sophistication degree of professional practices.

The first specific objective is establishing a general characterization of the available information on return of the Portuguese and Iberian direct real estate market nature and also a more specific one in terms of its segmentation structure. There is an intuitive and generalized perception that investors should use a structured approach to portfolio management for the maximization of results, which should be heavily conditioned by the common definitions of market segments. This raises questions on the actual level of reflection of systematic factors that effectively condition returns by the segment structures used in the Portuguese market. Results show that the structures based on Sector differentiation are generally significant and that regional spread does not condition property returns in the periods under study. This evidence supports the argument of Sector diversification, both in the Portuguese market and even in an enlarged Iberian context, similarly to the reality found by in similar research for the UK market.

The second objective is an analysis of the available Portuguese real estate indirect investment vehicles, the real estate investment fund

(REIF) industry, concerning its return related information, mostly in terms of distribution features, analysis and predictability. This study develops a detailed characterization of the most important available data on REIF performance, covering sources, base sample, construction methods and also a detailed analysis on the time series data as a basis for future research on performance prediction and attribution models, evaluating consistency, autocorrelation and explanatory relationships between variables and endogenous and exogenous factors. Strong evidence of behavioural heterogeneity across the industry and its subsectors is found. As for return distributions, evidence of non-normality is rather overwhelming, in line with previous findings for other real estate markets. Finally, persistence analysis using contingency tables is developed, in order to further develop on the issue of predictability. Relevant and robust evidence of both short and long term performance persistence within the overall property fund industry and for the restricted universe of open-ended funds was found.
Lastly, the third objective is portraying the sophistication level of current practices and decision-making processes used by the Portuguese organizations managing real estate as a financial asset, emphasizing on large portfolio holders. For this, a study based on a survey among a significant sample is developed. This includes REIF management societies, pension funds and large realty investment companies. The survey covers management decision-making practices, use of specific information, indices and databases, the role of appraisal, and the use of quantitative models to support diversification and asset allocation strategies, property selection decisions, performance measurement and benchmarking. The aim is to establish the real gap between theory, practical possibilities and real practice. Research design and results are presented and justified against economic reality, and recent similar studies in other markets.

02

ENGENHARIA DE ELECTRÓNICA DE TELECOMUNICAÇÕES E DE COMPUTADORES

Anuário Científico 2008

ISEL

AN EFFICIENT LONG DISTANCE ECHO CANCELLER

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This paper describes an implementation of a long distance echo canceller, operating on full-duplex with hands-free and in real-time with a single Digital Signal Processor (DSP). The proposed solution is based on short length adaptive filters centered on the positions of the most significant echoes, which are tracked by time delay estimators, for which we use a new approach. To deal with double talking situations a speech detector is employed. The floating-point DSP TMS320 C6713 from Texas Instruments is used with software written in C++, with compiler optimizations for fast execution. The resulting algorithm enables long distance echo cancellation with low computational requirements, suited for embedded systems. It reaches greater echo return loss enhancement and shows faster convergence speed when compared to the conventional approach. The experimental results approach the CCITT G.165 recommendation levels.

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Actas da ICSES'08 - International Conference on Signals and Electronic Systems, Cracóvia, Polónia, Setembro de 2008, pp 331-334. ISBN 978-83-88309-47-2, IEEE Catalog Number CFP0857D-PRT.

SUFFIX ARRAYS: A COMPETITIVE CHOICE FOR FAST LEMPEL-ZIV COMPRESSION

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Actas da SIGMAP'08- International Conference on Signal Processing and Multimedia Applications, Porto, Portugal, Julho de 2008, pp 5-12.

Lossless compression algorithms of the Lempel-Ziv (LZ) family are widely used in a variety of applications. The LZ encoder and decoder exhibit a high asymmetry, regarding time and memory requirements, with the former being much more demanding. Several techniques have been used to speed up the encoding process; among them is the use of suffix trees. In this paper, we explore the use of a simple data structure, named suffix array, to hold the dictionary of the LZ encoder, and propose an algorithm to search the dictionary. A comparison with the suffix tree based LZ encoder is carried out, showing that the compression ratios are roughly the same. The amount of memory required by the suffix array is fixed, being much lower than the variable memory requirements of the suffix tree encoder, which depends on the text to encode. We conclude that suffix arrays are a very interesting option regarding the tradeoff between time, memory, and compression ratio, when compared with suffix trees that make them preferable in some compression scenarios.

APPLICATION OF PML ABSORBING BOUNDARIES IN THE SPR METHOD

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The Finite-Difference Time-Domain (FDTD) method has been widely employed for the analysis and modelling of several structures and in the study of indoor and outdoor electromagnetic wave propagation [1]. However, its main advantages namely, simplicity and versatility, are obtained at the expense of significant computational resources. In particular, the simulation of realistic geometries may require a large simulation time. Recently, several variants have been proposed to improve the performance of Yee's original FDTD method. In this direction, we consider the Sparse Point Representation (SPR) method for the discretization of Maxwell's equations, which is a high order finite difference scheme combined with an interpolating wavelet adaptive strategy. The wavelet coefficients, defined in terms of local interpolation errors, can be regarded as indicators of the local smoothness of the fields. A thresholding procedure leads to grids that are sparse and nonuniformly spread: coarser in smooth regions and finer close to irregularities. This scheme provides a dynamically adapted grid with improved resolution in comparison to conventional time-domain schemes [2]. In previous simulations, we have used the SPR method to study the propagation of electromagnetic waves in homogeneous media. The main purpose of the present paper is to describe new developments concerning the inclusion of absorbing boundary conditions of Berenger perfectly matched layer (PML) type [1]. Illustrative numerical simulations of TE mode electromagnetic waves show that the solutions produced by the updated adaptive code and by the finite difference scheme in an uniform grid are in good agreement. The adaptive grid in the presence of the PML medium produces perturbations that are proportional to the threshold parameter.

RESOLUTION OF 2D MAXWELL'S EQUATIONS USING INTERPOLATING WAVELETS

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Publicado em:
VI Iberian Meeting on Computational Electromagnetics, Chiclana, Spain, 22-24 Outubro 2008.

Computational electromagnetic is a very active area and in the last decade there was a significant increase of its use for a wide class of applications. Yee's Finite-Difference Time-Domain (FDTD) method is a very useful numerical simulation technique for solving problems related to electromagnetism. This method is usually based in a uniform grid in which the electric and magnetic fields are described by vectors, both discretized in time and space. This can lead to a possible increase of the computation time. For this reason, it is important to study adaptive numerical methods that use a refined grid only in the regions of the space where the variation of the fields are intense, and a less refined grid in the other regions where the variation of the fields is smoother. The objective is to obtain an adaptive mesh as a function of time that allows to an economy of resources and a relatively short or acceptable time of simulation. This paper describes a method that combines a high order finite difference scheme for Maxwell's equations with an adaptive strategy based on interpolating technique, the so called Sparse Point Representation (SPR). Using this technique, the mesh structure presents a heterogeneous composition: sparse in smoothness regions and dense in regions of accented variation. The method combines the simplicity and accuracy of traditional finite difference schemes with the ability of wavelet coefficients in the characterization of local regularity of functions. In the present paper we demonstrate some of the potential of such scheme trough the results of the numerical simulation of a parallel-plate waveguide model with two irises.

FDTD COM ACTUALIZAÇÃO SELECTIVA: MÉTODO PARA MINIMIZAR O TEMPO DE SIMULAÇÃO

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A computação electromagnética teve nos últimos tempos um crescimento vertiginoso a que não está alheio o grande desenvolvimento que as comunicações móveis tiveram, nomeadamente com o aparecimento de diversos sistemas de comunicação móveis. Para que se possa fazer o projecto e análise destes sistemas de comunicação as ferramentas de simulação desempenham um papel fundamental e neste contexto o FDTD (Finite Difference Time Domain) surge como um dos métodos mais utilizados na simulação de propagação de ondas electromagnéticas quer em ambiente interior quer em ambiente exterior. No entanto dadas as exigências do método a simulação de uma determinada área tem uma complexidade computacional considerável. Neste artigo pretende-se comparar o tempo de simulação obtido entre o método convencional e o método com actualização selectiva. Para fazer este estudo utilizou-se um cenário fictício em 2D com uma área útil equivalente de 30mx30m. Os resultados gerados por ambos os métodos são comparados para permitir validar a técnica apresentada.

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IV Jornadas de Electrónica Telecomunicações e Computadores, Lisboa, Portugal, 20 e 21 de Novembro de 2008.

INFLUÊNCIA DA PRESENÇA HUMANA NO DESEMPENHO DE UMA ANTENA DE UM TERMINAL MÓVEL

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Publicado em:
IV Jornadas de Electrónica Telecomunicações e Computadores, Lisboa, Portugal, 20 e 21 de Novembro de 2008.

Neste artigo pretende-se analisar qual a influência que a presença humana, nomeadamente a cabeça, tem sobre os principais parâmetros de uma antena como o diagrama de radiação e o modulo do coeficiente de reflexão. De igual forma pretende-se determinar o nível de SAR (Specific Absortion Rate) imposto pelas antenas e verificar se os valores obtidos estão de acordo com os valores tabelados pelas normas. Para a realização deste estudo foram projectadas e medidas 3 antenas do tipo microstrip adequadas a um terminal móvel actual. Uma das antenas é adequada ao GSM 900, outra ao GSM 1800 e a terceira suporta simultaneamente os dois sistemas de comunicação anteriores. Posteriormente e por simulação usando um modelo de uma cabeça humana, foram determinados os níveis de SAR em diferentes situações, nomeadamente usando a antena com diferentes inclinações (0º, 45º e 90º) e a distâncias diferentes da cabeça (1,6 mm, 4,4 mm e 9,6 mm). De igual forma foram verificadas quais as alterações no diagrama de radiação e no módulo do coeficiente de reflexão que a presença humana impõe.

ANTENAS IMPRESSAS PARA TERMINAIS MÓVEIS PEQUENOS E MULTIBANDA

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Nesta publicação são apresentadas duas antenas PIFA impressas, de banda tripla e dimensões reduzidas. O comportamento multibanda é conseguido utilizando fendas em U. São ainda apresentadas dois novos tipos de fendas que permitem obter dimensões mais compactas. As antenas foram desenvolvidas de modo a suportarem os sistemas de comunicações móveis GSM900, GSM1800 e WLAN. Foram projectados, fabricados e medidos dois protótipos e obteve-se uma boa concordância entre os resultados teóricos e os resultados experimentais.

Publicado em:
5º Congresso Luso Moçambicano de Engenharia, Maputo, Moçambique, 02 a 04 de Setembro de 2008.

IDENTIFICAÇÃO DAS INTERACÇÕES DE SERVIÇOS PERSONALIZADOS

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Publicado em:
Quartas Jornadas de Engenharia Electrónica e Telecomunicações e de Computadores, Lisboa, 20 e 21 de Novembro de 2008.

A criação de novos serviços em aplicações Internet como correio electrónico ("Email"), telefonia sobre a Internet ("VoIP") e WWW levou à inevitável ocorrência de interacções, com comportamentos indesejáveis.
Nesta comunicação descreve-se a arquitectura e implementação dum simulador para identificação das interacções entre pares de serviços personalizados, subscritos por um utilizador.
Os serviços e personalizações são representados através dum modelo lógico sendo a detecção de interacções realizada por identificação de incoerências nas fórmulas lógicas. A identificação de incoerências auxilia o utilizador na escolha dos serviços a subscrever, evitando interacções.
A arquitectura do simulador assenta em tecnologia Java e teve como critérios de desenho: a riqueza funcional e facilidade de uso; o desempenho e a portabilidade.
São apresentados resultados experimentais do funcionamento do simulador em diversos cenários de interacção.

PLATAFORMA MULTI-AGENTE PARA AMBIENTE .NET (MA.NET)

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Este artigo apresenta de forma resumida a plataforma MA.NET, desenvolvida para permitir a construção de aplicações multi-agente conformes com as especificações da Foundation for Intelligent Physical Agents (FIPA) em ambiente .NET. São apresentados os objectivos do trabalho, descritos aspectos relevantes da implementação, avaliados os resultados e apontados trabalhos futuros. Dado tratar-se de um trabalho de implementação de um paradigma recente, ainda muito associado apenas à investigação, a ambientes de desenvolvimento tradicionais, espera-se que o trabalho contribua para acelerar o processo de migração desse paradigma para a indústria de software.

Publicado em:
Actas das Quartas Jornadas de Engenharia de Electrónica e Telecomunicações e de Computadores, ISEL, Novembro de 2008.

INTEREST RATE TERM STRUCTURE MODELLING FOR THE PORTUGUESE MARKET AND APPLICATIONS

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Publicado em:
Livro de Resumos de International Conference on Interdisciplinary Mathematical and Statistical Techniques - IMST 2008/FIM XVI, University of Memphis, Memphis, TN, USA, 16 a 18 de Maio de 2008.

We describe the Portuguese interest rate market, namely, the types of products for which a reliable pricing methodology is needed.
We next present two models for the discount function built upon the interest rates relevant for the Portuguese market. In the first approach the discount function is described by a cubic spline and in the second by a third degree polynomial, the coefficients being stochastic process for both the spline and the polynomial. The first model allows for the determination of a discount function with prescribed values at the maturities. The second model allows for forecasting. We discuss some preliminary results of the applications of these models.

INTEREST RATE MODEL SELECTION WITH GAUSSIAN PROCESSES

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We present an interest rate model selection method based on Gaussian Processes for machine learning.

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Livro de Resumos de International Conference on Interdisciplinary Mathematical and Statistical Techniques - IMST 2008/FIM XVI, University of Memphis, Memphis, TN, USA, 16 a 18 de Maio de 2008.

DYNAMIC RECOVERING OF LONG RUNNING TRANSACTIONS

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C. Kaklamanis and F. Nielson (Eds.): TGC 2008, LNCS 5474.

Most business applications rely on the notion of long running transaction as a fundamental building block. This paper presents a calculus for modelling long running transactions within the framework of the π-calculus, with support for compensation as a recovery mechanism. The underlying model of this calculus is the asynchronous polyadic π-calculus, with transaction scopes and dynamic installation of compensation processes. We add to the framework a type system which guarantees that transactions are unequivocally identified, ensuring that upon a failure the correct compensation process is invoked. Moreover, the operational semantics of the calculus ensures both installation and activation of the compensation of a transaction.

A SIMILARITY MEASURE FOR MUSIC SIGNALS

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

Publicado em:
Actas da 10th International Conference on Enterprise Information Systems, Barcelona, Espanha, 12 a 16 de Junho de 2008.

AN RNS BASED SPECIFIC PROCESSOR FOR COMPUTING THE MINIMUM SUM-OF-ABSOLUTE-DIFFERENCES

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Publicado em:
Actas do DSD'08-11th EUROMICRO CONFERENCE on DIGITAL SYSTEM DESIGN Architectures, Methods and Tools, Parma, Setembro de 2008, pp. 768-775.

The Sum of Absolute Differences (SAD) is a distance metric commonly used to determine the similarity between two data sets. A very recent method for directly comparing the magnitude of two numbers represented in Residue Number Systems (RNS) leads to the possibility of using modular arithmetic to compute the SAD. In this paper we propose an efficient hardware SAD unit that computes this Manhattan distance independently of each RNS channel. Therefore, the processing time can be reduced by simultaneously exploiting the carry-free characteristic of the modular arithmetic and the new method proposed by the authors of this paper to compare the magnitude of numbers in RNS. The proposed architecture is suitable to implement SAD units in Application Specific Integrated Circuit (ASIC) and in Field Programmable Gate Array (FPGA). In order to evaluate the performance of the proposed structures a hardware processor for computing the minimum SAD was implemented in a FPGA and ASIC. From the experimental results it was possible to obtain operating frequencies above 200 MHz for XILINX FPGAs XC2VP50-7 and XC4VLX80-12, and 300 MHz for the ASIC implementation. These results allow the implementation of real-time motion estimators for high resolution images according to the most recent standards for video coding.

TOWARDS BACKGROUND EMOTION MODELING FOR EMBODIED VIRTUAL AGENTS

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For the realistic simulation of embodied agents we need a model of emotion that represents both structural and dynamic aspects of emotional phenomena to serve as background support for multifaceted emotion characterization. In this paper we present an emotion model oriented towards that aim, which provides a continuous modeling of the evolution of emotional phenomena. We also illustrate how it can be used to provide different perspectives of an emotional situation, namely by identifying emotional patterns that can be characterized as discrete emotional states.

Publicado em:
Proceedings of the 7th International Joint Conference on Autonomous Agents and Multi Agent Systems, Lisboa, 12 a 16 de Maio de 2008, pp. 175-182.

ADVANCED SIDE INFORMATION CREATION TECHNIQUES AND FRAMEWORK FOR WYNER-ZIV VIDEO CODING

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Publicado em:
Journal of Visual Communication and Image Representation, Vol. 19, No. 8, December 2008, pp. 600-613.

Recently, several distributed video coding (DVC) solutions based on the distributed source coding (DSC) paradigm have appeared in the literature. Wyner–Ziv (WZ) video coding, a particular case of DVC where side information is made available at the decoder, enable to achieve a flexible distribution of the computational complexity between the encoder and decoder, promising to fulfill novel requirements from applications such as video surveillance, sensor networks and mobile camera phones. The quality of the side information at the decoder has a critical role in determining the WZ video coding rate-distortion (RD) performance, notably to raise it to a level as close as possible to the RD performance of standard predictive video coding schemes. Towards this target, efficient motion search algorithms for powerful frame interpolation are much needed at the decoder. In this paper, the RD performance of a Wyner–Ziv video codec is improved by using novel, advanced motion compensated frame interpolation techniques to generate the side information. The development of these type of side information estimators is a difficult problem in WZ video coding, especially because the decoder only has available some reference, decoded frames. Based on the regularization of the motion field, novel side information creation techniques are proposed in this paper along with a new frame interpolation framework able to generate higher quality side information at the decoder. To illustrate the RD performance improvements, this novel side information creation framework has been integrated in a transform domain turbo coding based Wyner–Ziv video codec. Experimental results show that the novel side information creation solution leads to better RD performance than available state-of-the-art side information estimators, with improvements up to 2 dB; moreover, it allows outperforming H.264/AVC Intra by up to 3 dB with a lower encoding complexity.

CONSTANT BITRATE CONTROL FOR A DISTRIBUTED VIDEO SYSTEM

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In some distributed video coding (DVC) systems, the total bitrate depends mainly on the key frames (Intra coded) quality and on the side information accuracy. In this paper, a rate control (RC) mechanism is proposed to achieve and maintain a certain target bitrate for the overall Intra and WZ bitstream, mainly by adjusting online the Intra frames quality through the quantization parameter (QP). In order to obtain a similar decoded quality of Intra and WZ frames, the relevant parameters: QP for the key frames and the quantization index (Q_{Index}) for WZ frames are controlled jointly. The major novelty of this work is a statistical model that expresses the relationship between Q_{Index} and WZ frames bitrate. The proposed rate control solution is integrated into the VISNET2 WZ codec and the experimental results demonstrate the efficiency of the proposed algorithm to reach and maintain the target bitrate.

Publicado em:
International Conference on Signal Processing and Multimedia Applications SIGMAP, Porto, Portugal, July 2008.

DESIGN AND PERFORMANCE OF A NOVEL LOW-DENSITY PARITY-CHECK CODE FOR DISTRIBUTED VIDEO CODING

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Publicado em:
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Low-density parity-check (LDPC) codes are nowadays one of the hottest topics in coding theory, notably due to their advantages in terms of bit error rate performance and low complexity. In order to exploit the potential of the Wyner-Ziv coding paradigm, practical distributed video coding (DVC) schemes should use powerful error correcting codes with near-capacity performance. In this paper, new ways to design LDPC codes for the DVC paradigm are proposed and studied. The new LDPC solutions rely on merging parity-check nodes, which corresponds to reduce the number of rows in the parity-check matrix. This allows to change gracefully the compression ratio of the source (DCT coefficient bitplane) according to the correlation between the original and the side information. The proposed LDPC codes reach a good performance for a wide range of source correlations and achieve a better RD performance when compared to the popular turbo codes.

WYNER-ZIV VIDEO CODING: A REVIEW OF THE EARLY ARCHITECTURES AND FURTHER DEVELOPMENTS

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In 2002, the video coding community faced the emergence of a new video coding paradigm, the so-called Wyner-Ziv video coding, which was represented by two early solutions designed by the Stanford University and the University of California, Berkeley research teams. This paper intends to briefly review, and compare these two early Wyner-Ziv video coding solutions, notably from the functional point of view. Moreover, this paper reviews some important developments of the Stanford Wyner-Ziv coding architecture, which has become the most popular in the literature.

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IEEE International Conference on Multimedia & Expo, Hannover, Alemanha, June 2008.

HIERARCHICAL MOTION ESTIMATION FOR SIDE INFORMATION CREATION IN WYNER-ZIV VIDEO CODING

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Publicado em:
The Second International Conference on Ubiquitous Information Management and Communication, Suwon, Korea, January 2008.

Recently, several video coding solutions based on the distributed source coding paradigm have appeared in the literature. Among them, Wyner-Ziv video coding schemes enable to achieve a flexible distribution of the computational complexity between the encoder and decoder, promising to fulfill requirements of emerging applications such as visual sensor networks and wireless surveillance. To achieve a performance comparable to the predictive video coding solutions, it is necessary to increase the quality of the side information, this means the estimation of the original frame created at the decoder. In this paper, a hierarchical motion estimation (HME) technique using different scales and increasingly smaller block sizes is proposed to generate a more reliable estimation of the motion field. The HME technique is integrated in a well known motion compensated frame interpolation framework responsible for the creation of the side information in a Wyner-Ziv video decoder. The proposed technique enables to achieve improvements in the rate-distortion (RD) performance up to 7 dB when compared to H.263+ Intra and 3 dB when compared to H.264/AVC Intra.

CODE CORRELATION REFERENCE WAVEFORMS FOR MULTIPATH MITIGATION IN MBOC GNSS

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The concept of code correlation reference waveforms (CCRW) for multipath mitigation in GPS receivers has been introduced by Lee. The CCRW is a train of specially tailored strobe pulses locked to the code sequence of the incoming signal. This approach is very powerful as most conventional delay lock loops are particular instances of CCRW. The wide application of the binary offset carrier (BOC) signals in modernized GPS and Galileo was the main motivation to extend the use of the concept of CCRW to BOC signals affected by multipath. In the sequel, the design of asymmetrical strobe pulses for BOC signals was proposed. Also, in the last years, several signal processing methods to reduce the effects of multipath have been proposed.

Recently, a joint design activity involving experts from the United States and Europe recommended an optimized multiplexed BOC modulation, MBOC(6,1,1/11), for the L1C signal and the Galileo E1 Open Service (OS) signal.

Following the previous work by the authors, this paper extends the CCRW concept to MBOC signals for the analysis and discussion of the multipath mitigation techniques performance in Global Navigation Satellite System (GNSS) BOC and MBOC receivers. Besides the comparison of the algorithms, a new approach for the S-curve design is introduced.

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Proceedings of European Navigation Conference, European Navigation Conference – Global Navigation Satellite Systems, April 23-25, Toulouse, France.

LEAST –SQUARES MINIMIZATION TECHNIQUE FOR MULTIPATH MITIGATION IN GNSS RECEIVERS

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Publicado em:
Proceedings of European Navigation Conference, European Navigation Conference – Global Navigation Satellite Systems, April 23-25, Toulouse, France.

Multipath is one of the major sources of positioning errors in GNSS receivers. Contrarily to other nuisances that affect the received signals, like the ionospheric and tropospheric delays, the effect of multipath on the computation of the pseudoranges cannot be usually attenuated by using pre-defined models. Many different signal processing techniques have been proposed to minimize the multipath problem with different degrees of success depending on the excess delay(s) of the secondary path(s) relative to the direct path of the incoming signal. In general, they fail to solve the problem for very short excess delays (typically smaller than 10 per cent of the chip duration). However, it is for this range of delays (close-in region) that the distortion suffered by the incoming signal may be stronger due to the power of the reflected signals.

Weil has shown that there is room for significant improvement in the performance of the multipath mitigation techniques operating in the close-in region if alternative approaches to the conventional techniques are considered. In the paper we propose a technique based in the nonlinear least-squares minimization using the vector of complex observations provided by a bank of correlators applied to the baseband version of the received signal. We adopted the Levenberg-Marquardt algorithm which is characterized by fast convergence and small computational burden for the problem in hands. However, other minimization algorithms could be used instead.

Following previous work, the proposed minimization technique in the present paper estimates a vector of parameters which includes the delays of the direct and the reflected ray, their amplitudes and relative phase.

BOC/MBOC MULTICORRELATOR RECEIVER WITH LEAST-SQUARES MULTIPATH MITIGATION TECHNIQUE

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The conventional techniques used for mitigating multipath in GNSS receivers, such as the Narrow Correlator or the High Resolution Correlator, present serious limitations in more complex multipath environments affected by several reflected rays. An alternative is to resort to algorithms, such as the Multipath Estimating Delay Lock Loop (MEDLL), that estimate the number, magnitude, delay and phase of the reflected rays. However, the weakness of the MEDLL is the steep increase of its computational burden with the number of reflected rays. Herein, we propose the application of the Levenberg-Marquardt (LM) algorithm to the code synchronization in multipath scenarios characterized by a large number of reflectors. The computational effort is kept at a reasonable level by assuming that the channel consists of a direct ray and a few reflectors despite the actual number of reflectors existing in the physical channel (in the paper we have considered 3 reflected rays for the LM algorithm). Simulations show a good robustness of the proposed algorithm in environments where the number of reflectors is large.

Publicado em:
Proceedings of the ION GNSS 2008, September 16-19, Savannah, Georgia, USA.

MULTIPATH MITIGATION TECHNIQUES IN MBOC GPS/GALILEO SIGNALS USING THE CCRW CONCEPT

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Publicado em:
Proceedings of NAVITEC 2008 – 4th ESA Workshop on Satellite Navigation User Equipment Technologies, 10-12 December, ESTEC, Noordwijk, The Netherlands.

A joint design activity involving experts from the United States and Europe recommended an optimized multiplexed Binary Offset Carrier (BOC) modulation, MBOC(6,1,1/11), for the GPS L1C signal and the Galileo E1 Open Service (OS) signal. This modulation is the result of multiplexing a narrow-band signal, BOC(1,1), with a wideband signal, BOC(6,1), in order to improve signal tracking performance. The additional contribution of the BOC(6,1) also aims at a higher intrinsic capability of limiting multipath effects. The Time Multiplexed BOC (TBOC) and the Composite BOC (CBOC) modulations adopted for L1C and E1 OS, respectively, are particular implementations of MBOC(6,1,1/11) using different approaches in the mixture of the BOC(1,1) and BOC(6,1) signals.

Following the previous work by the authors, this paper extends the CCRW concept to MBOC signals aiming the analysis and discussion of the multipath mitigation techniques performance in BOC and MBOC receivers. The algorithms are analyzed in terms of the tradeoff between multipath mitigation performance, robustness to thermal noise, and receiver bandwidth sensitivity. To extend the code tracking range, a new approach for the S-curve design is introduced. Innovative multipath mitigation techniques for MBOC receivers are also investigated.

CODE TRACKING ALGORITHM FOR GNSS OPEN-LOOP RECEIVERS USING AUTOCORRELATION INTERPOLATION

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Code tracking in conventional closed-loop receivers is implemented by a delay-lock loop with the discriminator response being around the null value for normal operation. This method is satisfactory for legacy GPS signals which exhibit a triangular autocorrelation; however, for modernized GNSS signals, namely BOC and MBOC, the autocorrelation is multipeaked leading to several nulls in the discriminator response (false code-locks).

The software solution herein proposed for non-coherent, low-cost receivers consists of heterodyning the incoming signal to baseband, sampling the resulting complex signal and performing the computation of a time-discrete version of the squared cross-correlation function from the noisy samples. The proposed interpolation technique is based on the reconstruction Sinc function, aiming to determine the position of the cross-correlation peak with a much smaller error than the one expected from the used sampling rate. Instead of relying on two samples and a linear interpolation formula to evaluate the peak, the new method uses a larger number of noisy samples provided by the correlators outputs, which are weighted by the Sinc function. This allows to improve the robustness to channel noise. Although the resulting pseudorange estimation algorithm is unbiased only for non-multipath environments, this technique can also be applied to multipath channels with good results, as shown in the simulations.

Publicado em:
Proceedings of NAVITEC 2008 – 4th ESA Workshop on Satellite Navigation User Equipment Technologies, 10-12 December, ESTEC, Noordwijk, The Netherlands.

TOWARDS NOISE CLASSIFICATION OF ROAD PAVEMENTS

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Publicado em:
Actas do EPAM 3rd European Pavement and Asset Management Conference, Coimbra, 7 e 9 de Julho de 2008, pp. 1-10.

Noise classification of road surfaces has been addressed in many European countries. This paper presents the first approach towards noise classification of Portuguese road pavements. In this early stage, it aims at establishing guidelines for decision makers to support their noise reduction policies and the development of a classification system adapted to the European recommendations. A ranking to provide guidance on tire-road noise emission levels for immediate use by decision makers, road authorities, contracting parties and environmental officers will be established. This research was based on the results provided by three early studies covering more than ten different surfaces, among which, rubberized asphalt and experimental non conventional surfaces with optimized grading. On each road trial, the tire-road noise generated by light vehicles and heavy trucks at three speed levels were measured by means of the Controlled Pass-By method (CPB). Three of these runs were also tested by the Close ProXimity method (CPX). Additionally, tests to characterize texture and skid resistance were performed. The early noise classification studies of road pavements focused only on the CPB tests. Three groups with similar acoustical performance were identified. Noise level abatements of about 10 dB were achieved for the gap graded mixtures with a maximum aggregate size inferior to 10 mm.

SILENT SURFACES: AN EXPERIENCE IN PORTUGAL

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It is acknowledged that traffic noise affects human behaviour and health. Measures aiming at mitigating the impact of traffic noise are not always viable in urban areas. In Portugal, road designers have recently started to consider silent surfaces as alternative within their road pavement projects. In this paper the tire-surface noise of three surface layers integrated in a rehabilitation project carried out in an urban road that carries more than 40000 vehicles per day is assessed: i) one dense asphalt layer with limited maximum aggregate size, following the SILVIA recommendations for low noise surfaces; ii) two very-thin surfaces with different grading, which are an adaptation of the very-thin layers widely used in France to Portuguese conditions. The surface layers were constructed consecutively, involving segment lengths with more than 500 m. The surface texture was measured using a high speed profilometer. Skid resistance was also measured. The noise level was measured both by pass-by tests with selected traffic (trucks and light vehicles) at several speeds and by close proximity tests. The thin layers tested provided very good noise reduction values, especially at high speeds, and had a better performance than gap graded asphalt rubber surfaces frequently used in Portugal.

Publicado em:
Actas do SURF 6th Symposium on Pavement Surface Characteristics, Portoroz, Eslovénia, 20 e 22 de Outubro de 2008, pp. 1-15.

A HYBRID MLS TECHNIQUE FOR ROOM IMPULSE RESPONSE ESTIMATION

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Applied Acoustics, 2008 (online) - doi:10.1016/j.apacoust.2008.07.007, 2009 (revista), Volume 70, Issue 4, 556-562.

The measurement of Room Impulse Response (RIR) when there are high background noise levels frequently means one must deal with very low signal to noise ratios (SNR). If such is the case, the measurement might yield unreliable results, even when synchronous averaging techniques are used. Furthermore, if there are non-linearities in the apparatus or system time-variances, the final SNR can be severely degraded. The test signals used in RIR measurement are often disturbed by non-stationary ambient noise components. A novel approach based on the energy analysis of ambient noise - both in the time and in frequency - was considered. A modified Maximum Length Sequence (MLS) measurement technique, referred to herein as the Hybrid MLS technique, was developed for use in room acoustics. The technique consists of reducing the noise energy of the captured sequences before applying the averaging technique in order to improve the overall SNRs and frequency response accuracy. Experiments were conducted under real conditions with different types of underlying ambient noises. Results are shown and discussed. Advantages and disadvantages of the Hybrid MLS technique over standard MLS technique are evaluated and discussed. Our findings show that the new technique leads to a significant increase in the overall SNR.

STATISTICAL LEARNING METHODS APPLIED TO ROAD PAVEMENT CLASSIFICATION

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The measurement procedure to evaluate the influence of road surface characteristics on vehicle and traffic noise is designated by Close-Proximity (CPX) method, as described in the ISO 11819-2 draft. This procedure consists on acquiring the vehicle rolling noise signal near the tires and close to the surface by means of at least two microphones in a special arrangement. The main goal of this research is to identify and classify different types of road pavements by analyzing the near field sound profile using Statistical-learning methods. Feature extraction and selection is one of the first procedures on a classifier system. Moreover, the accuracy of the results is strongly dependent on the choice of the selected feature vector. An important issue of road pavement classification regards the improvement of the quality of road traffic data in order to increase the accuracy of the road noise mapping models. Results based on the probability of costly errors are presented and discussed. The resulting approach is evaluated with respect to classification accuracy and computational cost.

Publicado em:
Actas de Acústica 2008 – V Congresso Ibérico de Acústica, Coimbra, 20 e 22 de Outubro de 2008, pp. 1-10.

UNVEILING INTRINSIC SIMILARITY: APPLICATION TO TEMPORAL ANALYSIS OF ECG

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Publicado em:
Actas da Bio-inspired Systems and Signal Processing - Biosignals08 part of Int'l Joint Conf. on Biomedical Engineering Systems and Technologies, Funchal, Janeiro 2008.

The representation of data in some visual form is one of the first steps in a data-mining process in order to gain some insight about its structure. We propose to explore well known visualization and unsupervised learning techniques, namely clustering, to improve the understanding about the data and to enhance possible relations or intrinsic similarity between patterns. Specifically, Clustering Ensemble Methods are exploited separately and combined to provide a clearer visualization of data organization. The presented methodology is used to improve the understanding of ECG signal acquired during Human Computer Interaction (HCI).

ESTUDO EXPLORATÓRIO PARA ORGANIZAÇÃO AUTOMÁTICA DE MENSAGENS DE CORREIO ELECTRÓNICO

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A organização automática de documentos de texto, particularmente de mensagens de correio electrónico (*e-mails*), apresenta-se com um problema muito actual e de grande interesse prático. Este artigo apresenta um estudo, onde técnicas de *Text Mining* são aplicadas de uma forma exploratória no contexto de uma aplicação real - a organização automática das mensagens de correio electrónico processadas durante a realização de uma conferência ciêntifica pelo INSTICC (*Institute for Systems and Technologies of Information, Control and Communication*). São estudadas diferentes formas de representação dos documentos - desde a clássica representação *tf-idf*; a técnicas como o *latent semantic indexing*; à utilização de conhecimento a *priori* usando a rede semântica *WordNet* – e de forma sistemática verificada a sua influência no agrupamento automático de mensagens usando técnicas de *clustering*, nomeadamente as clássicas k-médias. Os resultados preliminares demonstram o interesse do estudo e a possível utilização destas técnicas em contexto real.

Publicado em:
Actas da JETC'08, Lisboa, Novembro 2008.

DETECÇÃO DE ANOMALIAS EM LINHAS DE ALTA TENSÃO

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Publicado em:
Actas da JETC'08 IV Jornadas de Engenharia Electrónica e Telecomunicações e de Computadores, Lisboa, Novembro de 2008, pp. 111-116.

Este artigo apresenta uma nova abordagem para processamento em tempo-real de um sistema de detecção de anomalias em linhas de alta tensão, permitindo a detecção automática destas. Utiliza algoritmos de clustering para a detecção da linha e das anomalias. Através dos resultados experimentais é demonstrada a possibilidade de detecção em tempo-real num DSP - TMS320C6713 DSK da Texas Instruments.

EVALUATION OF COLLABORATIVE ANNOTATION SYSTEMS AND SIMULATION OF USER BEHAVIOR ON SOCIAL NETWORK

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In this paper we propose an approach for modeling the user annotation behavior based on a simulated query feedback. The annotation skills are the basis for the collaborative annotation systems, which compare the users' information needs (expressed in a query), with the annotations (made by users) that classify the documents. The evaluation of annotation systems is complex due to: i) the difficulty in closing the environment, ii) the number and diversity of users, and iii) the language subjectivity. Our simulation explores the relation between the user society and their annotation skills to better understand how it affects the systems' retrieval accuracy. This approach can also be applied to measure the systems performance in information retrieval systems.

Publicado em:
Proceedings of 1st. Brazilian Workshop on Social Simulation in the the 19th Brazilian Symposium on Artificial Intelligence.

DA MODELAÇÃO À AUTOMAÇÃO DE PROCESSOS NO DESENVOLVIMENTO DE NOVOS PRODUTOS

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Publicado em:
Actas da 8ª Conferência da Associação Portuguesa de Sistemas de Informação (CAPSI), 29 a 31 de Outubro 2008, Setúbal.

Este trabalho tem por objectivo permitir a redução do tempo de desenvolvimento de um produto tão complexo como é um automóvel. É apresentado um modelo iterativo que permite realizar análises relacionadas com aspectos de homologação e ergonomia. Todas as actividades relacionadas com o desenvolvimento do produto serão modeladas e optimizadas recorrendo ao UML (Unified Modeling Language) através de uma linguagem derivada, designada por VDML (Vehicle Development Modeling Language). As actividades são descritas por modelos, os quais representam a realidade de uma forma simplificada. Estes modelos são usados para a criação automática de código, o qual é embebido num ambiente paramétrico CAD/CAS de forma a automatizar regras de ergonomia e homologação.

KAD – AN INTEGRATED CAD AND CSCW SYSTEM FOR THE DEVELOPMENT OF NEW PRODUCT IN INDUSTRY BUSINESS

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This paper defines the KAD's architecture, an integrated CAD and CSCW system, for better support the design process in industry, particularly on the development of new products in automotive sector. The KAD system intends to reduce the lead time by providing and integrating flexible and efficient capabilities for testing early concepts from the ergonomic, surface analysis and normative points of view in automotive product development. Based on domain ontology and on information repository we define tools for knowledge management and retrieval of technical knowledge via models in new CAD environment, helping the users to perform their job. These characteristics differentiate the KAD system from others, because it supports intelligent rules engine, for extrapolate and make inference with historical surfaces and solutions that allow the generation of technical surfaces, the use of ergonomics and homologation rules and also the automatic integration of automatic job routines in CAD.

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Proceedings of 6th IEEE International Conference on Industrial Informatics INDIN 2008, July 13-16, 2008 in Daejeon - Korea.

SIMILARIDADE SEMÂNTICA BASEADA EM TAXIONOMIAS

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Publicado em:
Publicado nos proceedings das Jornadas de Engenharia de Electrónica e Telecomunicações e de Computadores (JETCø8), ISEL, 20 a 21 Novembro de 2008.

Este artigo apresenta uma abordagem para calcular as medidas de similaridade semântica entre conceitos dado uma hierarquia de conhecimento (e.g taxionomia, ontologia). Deste processo resulta um grafo de conceitos, onde as relações semânticas entre conceitos são representadas graficamente por um arco, onde o peso do arco traduz o valor da medida de similaridade entre um par de conceitos. O peso do arco é determinado é função da medida de similaridade aplicada. A abordagem proposta é aplicável, por exemplo, quando se pretende enriquecer modelos de domínio definidos por conceitos que desempenham o papel de unidades atómicas de conhecimento. Concretamente, é referido como caso de estudo o modelo de domínio dos sistemas de diálogo. Neste âmbito, constata-se que os arcos de similaridade melhoram a contribuição do modelo do domínio para apoiar e tornar mais eficazes as estratégias de diálogo concebidas para explorar a similaridade entre conceitos, designadamente na condução de diálogos de clarificação.

SISTEMA DE RECUPERAÇÃO DE OBJECTOS DIGITAIS

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O presente artigo propõe a concepção de um sistema de recuperação de informação de diversos Objectos Digitais (OD) com recurso a metadados descritivos do objecto (dados que descrevem outros dados). Para fomentar o processo de preenchimento dos metadados é proposto um mecanismo de créditos para estimular o preenchimento cooperativo entre utilizadores e autores de OD's., com base na metáfora da bolsa de valores. Deste processo de anotações resulta incerteza associado a subjectividade humana da linguagem, ou seja, para o mesmo objecto podem existem várias descrições, que podem ser interpretadas de formas diferentes, pelo que será proposto um modelo de determinação da relevância de um OD e do peso dos termos dos metadados necessários para a criação de uma Base de dados (BD) probabilística.

Publicado em:
Publicado nos proceedings das Jornadas de Engenharia de Electrónica e Telecomunicações e de Computadores (JETCø8), ISEL, 20 a 21 Novembro de 2008.

PLATAFORMA AVANÇADA DE DESENHO AUTOMÓVEL

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Publicado em:
Revista CAD Project - Ibéria Editora em Janeiro 2008.

Este trabalho tem por objectivo permitir a redução do tempo de desenvolvimento de um produto tão complexo como é um automóvel. É apresentado um modelo iterativo que permite realizar análises relacionadas com aspectos de homologação e ergonomia. Todas as actividades relacionadas com o desenvolvimento do produto serão modeladas e optimizadas recorrendo ao UML (Unified Modeling Language) através de uma linguagem derivada, designada por VDML (Vehicle Development Modeling Language). As actividades são descritas por modelos, os quais representam a realidade de uma forma simplificada. Estes modelos são usados para a criação automática de código, o qual é embebido num ambiente paramétrico CAD/CAS de forma a automatizar regras de ergonomia e homologação.

SISTEMA DE PESQUISA DE INFORMAÇÃO MULTIMÉDIA

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O presente trabalho propõe a concepção de um sistema de pesquisa de informação de objectos multimédia com recurso a metadados descritivos.
Para fomentar o processo de preenchimento dos metadados, é proposto um mecanismo de créditos para estimular o preenchimento cooperativo entre utilizadores e autores, com base na metáfora da bolsa de valores. Deste processo de anotações resulta incerteza associada à subjectividade da linguagem humana, ou seja, para o mesmo objecto podem existir várias descrições. Por sua vez estas podem ser interpretadas de formas diferentes, pelo que será proposto um modelo de determinação da relevância de um objecto digital e do peso dos termos dos descritivos. Este modelo é necessário para a criação de um repositório de metainformação.

Publicado em:
RISTI (Revista Ibérica de Sistemas e Tecnologias de Informação) em Julho de 2008.

KC-PLM: KNOWLEDGE COLLABORATIVE PRODUCT LIFECYCLE MANAGEMENT

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Publicado em:
Handbook of Research on Social Dimensions of Semantic Technologies and Web Services. (http://handbooksemanticweb.ipca.pt)

This paper defines a system and a methodology, the Knowledge Collaborative Product Lifecycle Management (KC-PLM) to better support the complete product lifecycle in the industry. The KC-PLM system intends to reduce the lead-time from new product development to production by providing and integrating knowledge platform, based on a semantic information repository, domain ontology, a domain specific language and on the user collaboration. These characteristics differentiate the KC-PLM system from others PLM systems, because it supports an intelligent rules engine, to extrapolate and make inference with historical solutions that allow the generation of new solutions. A real case study in automobile business shows the current proposal application and its benefits in a product concept phase.

EMPIRICAL MULTI-ARTIFACT KNOWLEDGE MODELING FOR DIALOGUE SYSTEMS

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This paper presents a knowledge modeling approach to improve domain-independency in Spoken Dialogue Systems (SDS) architectures. We aim to support task oriented dialogue management strategies via an easy to use interface provided by an adaptive Domain Knowledge Manager (DKM). DKM is a broker that centralizes the knowledge of the domain using a Knowledge Integration Process (KIP) that merges on the fly local knowledge models. A local knowledge model defines a semantic interface and is associated to an artifact that can be a household appliance in a home domain or a cinema in a ticket-selling domain. We exemplify the reuse of a generic AmI domain model in a home domain and in a ticket-selling domain redefining the abstractions of artifact, class, and task. Our experimental setup is a domain simulator specially developed to reproduce an Ambient Intelligence (AmI) scenario.

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02

DIALOGUE SYSTEMS DOMAIN INTERACTION USING REINFORCEMENT LEARNING

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Publicado em:
11th Ibero-American Conference on Artificial Intelligence - Workshop on Agreement Technologies, 2008.

This paper describes research about using a reinforcement learning approach to optimize our Domain Knowledge Manager (DKM) that is part of a mixed-initiative task based Spoken Dialogue System (SDS) architecture, namely to access an Ambient Intelligence (AmI) scenario. Assuming that practical dialogue and domain-independent hypothesis are true, we have considered a clear separation between discourse dependent and domain dependent knowledge, which allows reducing the complexity of SDS typical components, specially the Dialoguer Manager (DM). In this context, we believe that is possible to get better DM strategies optimizing the interaction between DM and DKM. For this, we propose a new feature, for the DKM, based on learning and suggest the best task artifact pairs to satisfy a DM query using the DM feedback as reward. The proposed DKM feature has been tested in our simulator based on Portuguese language.

ACTUALIZAÇÃO DE CONHECIMENTO EM SISTEMAS DE DIÁLOGO

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Este artigo descreve uma abordagem para melhorar o conhecimento representado no modelo do domínio de um Sistema de Diálogo (SD). Um SD permite ao seu utilizador interactuar, através de fala, por exemplo, com um Ambiente Inteligente (AmI) composto por um conjunto de artefactos heterogéneos. Tipicamente, as tarefas disponibilizadas ao utilizador são representadas no modelo do domínio fazendo referências a unidades atómicas de conhecimento, designadas por conceitos. A actualização de conhecimento proposta sugere a inserção de arcos de similaridade, entre pares de conceitos, representados por descritores e determinados por métricas de similaridade. É apresentado um estudo de caso sobre alimentos.

Publicado em:
14th WebMedia - 6th Workshop in Information and Human Language Technology, 2008.

LEVEL SHIFTERS AND DCVSL FOR A LOW-VOLTAGE CMOS 4.2-V BUCK CONVERTER

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Publicado em:
IEEE Transactions on Industrial Electronics, 2008, Vol. 55, No9, 3315-3323.

In this paper, high-voltage (HV)-tolerant level shifters with combinational functionality are proposed based on differential cascode voltage switch logic (DCVSL). These level shifters are tolerant to supply voltages higher than the process limit for individual CMOS transistors. The proposed HV DCVSL level shifters are particularly useful when it is mandatory to constrain the output using a logic function during out of the normal mode periods (power-up, power-down, reset, etc.). These HV-tolerant logic circuits were used in the power block of a buck converter designed in a standard 3.3-V 0.13-µm CMOS process, powered by an input voltage range from 2.7 to 4.2 V. Simulation and experimental results of the buck are analyzed, and the topology is evaluated.

NOME DA COMUNICAÇÃO EM MAÍSCULAS E SEMPRE NESTE FORMATO DE LETRA

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Resumo do artigo em tamanho de letra 12, times news roman a um espaço e respeitando as margens já definidas e máximo duas paginas.

Publicado em:
Journal of Chemical and Computacional Education, 2001, 46, 123-127.

RECONHECIMENTO AUTOMÁTICO DE ORADOR

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Publicado em:
Quartas Jornadas de Engenharia de Electrónica e Telecomunicações e de Computadores – JETCø8, 2008, actas em formato CD.

Descrevemos e comparamos dois sistemas de verificação de orador, um utilizando um classificador "support vector machines" (SVM) e outro utilizando "*universal background model Gaussian mixture models*" (UBM-GMM). Nestes dois sistemas foram testados diversos parâmetros dos sinais de fala: "*mel frequency cepstral coefficients*" (MFCC), "line spectrum frequencies" (LSF) e "*mel line spectrum frequencies*" (MLSF). Os parâmetros MLSF resultam na introdução de informação perceptiva nos tradicionais LSF, visando melhorar a taxa de reconhecimento e continuando a gozar das propriedades de codificação dos LSF, podendo ser directamente transmitidos com eficiência sem que seja necessário transmitir o sinal de fala e assim abrir caminho para a autenticação remota. Foram ainda implementadas técnicas de normalização de resultados: a normalização "*zero normalization*" Z-norm e a normalização "*target normalization*" (T-norm). A avalização dos sistemas foi realizada com base no "*equal error rate*" (EER) e no valor mínimo do CDET. Os testes foram efectuados nos corpora 2001 e 2002 NIST SRE.

IMPROVEMENT IN PINPIN DEVICE ARCHITECTURES FOR IMAGING APPLICATIONS

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The effect of the applied voltage on the color selectivity is discussed. Results show that the spectral response curves demonstrate rather good separation between the red, green and blue basic colors. Combining the information obtained under positive and negative applied bias a colour image is acquired without colour filters or pixel architecture. A low level image processing algorithm is used for the colour image reconstruction.

Publicado em:
Actas da Material Research Society Spring Meeting, Simpósio A: Amorphous and Polycrystalline Thin-Film Silicon Science and Technology, S. Francisco, E.U.A., 24 a 28 de Março de 2008, vol. 1066, A18-02.

MULTILAYERED A-SIC:H DEVICE FOR WAVELENGTH-DIVISION (DE) MULTIPLEXING APPLICATIONS IN THE VISIBLE SPECTRUM

Vieira, M.[1,2]; Fernandes, M.[1]; Louro, P.[1,2]; Vieira, M.A.[1,3]; Barata, M.[1,2]; Fantoni, A.[1]

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Publicado em:
Actas da Material Research Society Spring Meeting, Simpósio A: Amorphous and Polycrystalline Thin-Film Silicon Science and Technology, S. Francisco, E.U.A., 24 a 28 de Março de 2008, vol. 1066, A08-01.

A multiplexer is a device that combines two or more signals onto a single output without losing their specificity. In this paper we present results on the use of multilayered a-SiC:H heterostructures either as wavelength-division multiplexing or demultiplexing device (WDM). The WDM is a glass/ITO/a-SiC:H (p-i-n)/ a-SiC:H(-p) /Si:H(-i')/SiC:H (-n')/ITO double heterostructure which faces the modulated light incoming together from different beams. The input beams are absorbed accordingly to its wavelength giving rise together to a time dependent wavelength electrical field modulation across the device. By reading out, at different applied bias, the photocurrent generated by all the incoming optical carriers, the information is multiplexed or demultiplexed and can be transmitted and recovered again. The devices were characterized through spectral response measurements, under different electrical bias and frequencies. Results show that in the multiplexing mode the output signal is balanced by the wavelength of each incoming optical carrier and modulated by their frequencies. In the demultiplexing mode the photocurrent is controlled by the applied voltage and optical bias allowing to regain the transmitted information. An electrical model is presented to explain the WDM device operation.

NON-SELECTIVE OPTICAL WAVELENGTH-DIVISION MULTIPLEXING DEVICES BASED ON A-SIC:H MULTILAYER HETEROSTUCTURES

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In this paper we present results on the optimization of multilayered a-SiC:H heterostructures for wavelength-division (de) multiplexing applications. The non selective WDM device is a double heterostructure in a glass/ITO/a-SiC:H (p-i-n) /a-SiC:H(-p) /a-Si:H(-i')/a-SiC:H(-n')/ ITO configuration. The single or the multiple modulated wavelength channels are passed through the device, and absorbed accordingly to its wavelength, giving rise to a time dependent wavelength electrical field modulation across it. The effect of single or multiple input signals is converted to an electrical signal to regain the information (wavelength, intensity and frequency) of the incoming photogenerated carriers. Here, the (de) multiplexing of the channels is accomplished electronically, not optically. This approach offers advantages in terms of cost since several channels share the same optical components; and the electrical components are typically less expensive than the optical ones. An electrical model gives insight into the device operation.

Publicado em:
Actas da Material Research Society Spring Meeting, Simpósio K: Materials and Devices for Laser Remote Sensing and Optical Communication, S. Francisco, E.U.A., 24 a 28 de Março de 2008, vol. 1076, K098-02.

TRANSIENT CURRENT IN A-SI:H-BASED MIS PHOTOSENSORS

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Publicado em:
Actas da Material Research Society Spring Meeting, Simpósio A: Amorphous and Polycrystalline Thin-Film Silicon Science and Technology, S. Francisco, E.U.A., 24 a 28 de Março de 2008, vol. 1066, A18-06.

In this work we analyze the transient current in the metal/a-SiNx/a-Si:H/n+/ITO structures under different biasing conditions and temperatures. The dark current decay was measured within an interval of 1 second in the temperature range from 294 to 353K. It was found that when the bias pulse amplitude is kept constant, the transient current strongly depends upon the offset voltage of the bias pulse. This result is in good agreement with device modeling performed using ATLAS. The detailed analysis shows that the transient dark current originates from traps in the i-layer bulk and traps at the semiconductor-insulator interface. Under optimized biasing conditions and elevated temperatures the bulk current component becomes dominant.

DEMULTIPLEXAGEM ÓPTICA CONTROLADA POR TENSÃO NO DOMÍNIO DO VISÍVEL

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Nesta comunicação pretende-se caracterizar um sistema multiplexer/demultiplexer usando uma estrutura pi-n baseada em a-Si:H e/ou a-SiC:H que funciona como sensor de cor e utiliza como meio de transmissão a fibra óptica. O propósito é obter o sinal óptico conhecido que irá passar pelas diferentes fases de multiplexagem e demultiplexagem, no domínio dos comprimentos de onda da luz visível (WDM-Wavelength-division multiplexing).

Publicado em:
Livro de Actas das Jornadas do JETCø8, IV Jornadas de Electrónica e das Telecomunicações, 20 a 21 de Novembro de 2008, ISEL, Lisboa (www.deetc.isel.ipl.pt/jetcø8, ISBN 978-972-95809-4-9).

PROJECTO DE NOVAS TECNOLOGIAS DE SEMÁFOROS RODOVIÁRIOS

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Publicado em:
Livro de Actas das Jornadas do JETCø8, IV Jornadas de Electrónica e das Telecomunicações, 20 a 21 de Novembro de 2008, ISEL, Lisboa (www.deetc.isel.ipl.pt/jetcø8, ISBN 978-972-95809-4-9).

Um novo desafio surge com a aplicação de LEDs no controlo automático de tráfego. Serão propostas novas soluções que passam por novas regras de localização, recurso a novas técnicas de animação, possibilidade de utilização de informação adicional para condutores e peões, possibilidade de utilização de novos semáforos dirigidos a camadas específicas de utilizadores como os veículos de socorro e bombeiros. Na rede viária envolvente aos túneis rodoviários urbanos, associado à necessidade de introdução de corredores de segurança, o módulo prioridade aos veículos de bombeiros compreenderá software adicional nas acções de microregulação utilizando "novos semáforos SOS" equipados com LED'S (Light Emitting Diodes) e ligações aos detectores de prioridade instalados na via pública.

GESTÃO INTEGRADA DE UM TÚNEL EM MEIO URBANO

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Os túneis rodoviários urbanos são, nos dias de hoje, estruturas fundamentais na gestão do tráfego. Neste trabalho pretende-se demonstrar como esse objectivo pode ser atingido, implementando regras e procedimentos de segurança que, de uma maneira racional, nos conduzam à melhor regulação possível do tráfego, em cada momento.

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Livro de Actas das Jornadas do JETCø8, IV Jornadas de Electrónica e das Telecomunicações, 20 a 21 de Novembro de 2008, ISEL, Lisboa (www.deetc.isel.ipl.pt/jetcø8, ISBN 978-972-95809-4-9).

SELF-BIASING EFFECT IN COLOUR SENSITIVE PHOTODIODES BASED ON DOUBLE P-I-N A-SIC:H HETEROJUNCTIONS

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Publicado em:
Vacuum, 2008, 82, 1512-1516.

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)/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 show that the 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 it 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 colour filter analysis.

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

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This work reports on the fabrication and characterization of indium oxide semiconducting films and their application in thin-film transistors (TFTs). The films have been deposited at room temperature by oxygen ion beam assisted e-beam evaporation. The influence of deposition conditions on film properties including the crystal structure, conductivity, and intrinsic stress is analyzed. It is found that the electrical properties of indium oxide films can be engineered from metallic to insulating and the film structure can be varied from amorphous to microcrystalline by adjusting deposition rate, oxygen ion energy, and ion beam flux. Furthermore, the highly-resistive films with considerable microstructural crystallinity exhibit n-type field-effect behaviour. A field-effect mobility of 1.4 cm2/V s, and ON/OFF current ratio of 106 are observed for transistors with a silicon dioxide gate dielectric.

Publicado em:
Physica Status Solidi A-applications and Materials Science, 2008, 205, 1925-1928.

02

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

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Publicado em:
Physica Status Solidi A-applications and Materials Science, 2008, 5, 3410-3413.

This paper reports on a method and a test setup developed to measure the transient dark current and the spectral response characteristics of a-Si:H MIS photosensors. Using this method the segmented-gate/SiNx/a Si:H/n+/ITO structures have been characterized under different biasing conditions. The dependences of the dark and light signals on the refresh pulse amplitude, offset voltage and pulse width were measured and analyzed. It is found that the amplitude of the time-dependent component of the leakage current associated with charge trapping at the insulator-semiconductor interface can be significantly reduced by adjusting the offset voltage. The observed bias dependence of the spectral response characteristics is explained by analyzing the charge carrier transport in the absorption layer at different wavelengths of the incident light.

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

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It is presented in this paper a study on the photo-electronic properties of multilayer a-Si:H/a-SiC:H p-i-n-i-p structures. This study is aimed to give an insight into the internal electrical characteristics of such a structure in thermal equilibrium, under applied bias and under different illumination condition. Taking advantage of this insight it is possible to establish a relation among the electrical behavior of the structure, the structure geometry (i.e. thickness of the light absorbing intrinsic layers and of the internal n-layer) and the composition of the layers (i.e. optical bandgap controlled through percentage of carbon dilution in the a-Si1-x Cx:H layers).

Showing an optical gain for low incident light power con- trollable by means of externally applied bias or structure composition, these structures are quite attractive for photo-sensing device applications, like color sensors and large area color image detector.

An analysis based on numerical ASCA simulations is presented for describing the behavior of different configurations of the device and compared with experimental measurements (spectral response and current-voltage characteristic).

Publicado em:
Physica Status Solidi A-applications and Materials Science, 2008, 205, 2069-2074.

PHOTOCAPACITANCE MEASUREMENTS IN IRRADIATED A-SI:H BASED DETECTORS

Schwarz, R.[1]; Mardolcar, U.[1]; Vygranenko, Y.[2]; Vieira, M.[2]; Casteleiro, C.[3]; Stallinga, P.[3]; Gomes, H.[3]

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Publicado em:
Journal of Non-Crystalline Solids, 2008, 354, 2176-2180.

Photocapacitance measurements were performed on amorphous silicon p-i-n detectors before and after particle irradiation with 1.5 MeV 4 He+ ions. The spatial resolution across a degraded spot is similar to the one obtained in photocurrent scans and is of the order of the diameter of the scanning laser beam. We monitored the transient capacitance after applying short laser pulses to deduce trap energies of 0.64 eV. Photocapacitance measurements as a function of the applied bias, the measurement frequency up to 1 MHz, and the wavelength of laser light are discussed. The reduction in photocapacitance signal and the shift of the cut-off frequency after ion bombardment are correlated with the change in transport properties.

SPATIALLY-RESOLVED PHOTOCAPACITANCE MEASUREMENTS TO STUDY DEFECTS IN A-SI:H BASED P–I–N PARTICLE DETECTORS

Casteleiro, C.[1]; Schwarz, R.[1]; Mardolcar, U.[1]; Maçarico, A.[2]; Martins, J.[2]; Vieira, M.[2]; Wuensch, F.[3]; Kunst, M.; Morgado, E.[4]; Stallinga, P.[5]; Gomes, H.L.[5]

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Thick large-area particle or X-ray detectors suffer degradation during operation due to creation of defects that act as deep traps. Measuring the photocurrent under homogeneously absorbed weak light can monitor variation in detector performance. We describe how photocapacitance can be used as an alternative method to measure the creation of defects and their energy level after intense irradiation with protons or He ions at 1.5 MeV and after exposure to intense laser pulses. The possibility to detect small areas of high defect density in a large-area detector structure is discussed.

Publicado em:
Thin Solid Films, 2008, 516, 5118-5121.

PERFORMANCE OF A-SI : H N-I-P PHOTODIODES ON PLASTIC SUBSTRATE

Kim, K.H.[2]; Vygranenko, Y.[1]; Striakhilev, D.[2]; Bedzyk, M.[3]; Chang, J.H.[2]; Nathan, A.[4]; Chuang, T.C.[2]; Heiler, G.[3]; Tredwell, T.[3]

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Publicado em:
Journal of non-crystalline solids, 2008, 354, 19-25.

This paper reports on a-Si:H n-i-p photodiodes on PEN substrates with performance characteristics suitable for imaging applications. Segmented n-i-p photodiodes were fabricated using a process sequence and design rules that are compatible with industrial technology. Low-temperature (150 degrees C) plasma-enhanced chemical vapor deposition (PECVD) was employed for the a-Si: H and passivation dielectric layers. Device measurements included current-voltage characteristics, dark current decay, and spectral response. To identify the sources of the reverse dark current, the measurements were performed on variable area test structures with device sizes ranging from 126 mu m to 2 mm. The n-i-p photodiodes on PEN substrates demonstrate quantum efficiencies as high as 83% and reverse current density lower than 500 pA/cm(2) at -3 V, as measured on 126 mu m photodiodes. Thus, the performance characteristics of the n-i-p diodes on PEN substrates meet the requirements for bio-medical X-ray imaging. We also discuss the mechanisms underlying the reverse dark current and the effect of the substrate on device characteristics.

MONOLITHIC PINPIN HETEROJUNCTIONS FOR IMAGE AND COLOUR IMAGE RECOGNITION

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In this paper we present results on the optimization of device architectures for color and imaging applications. The sensor is a stacked device composed by a glass/ITO/p-i-n a-SiC:H photodiode for image reading followed by a-SiC:H(-p) /Si:H(-i')/SiC:H (-n')/ITO heterostructure that works as the reading element. The doped layers are based on a-SiC:H to increase image resolution and to prevent image blurring. The intrinsic layer of the front diode is thinner and based on a-SiC:H while the back one is thicker and based on a-Si:H. The photocurrent generated by the optical scanner gives information on the image intensity levels. For colour image acquisition, different sensitivity spectral ranges are selected by using a voltage scan waveform and a reconstruction low level image processing algorithm allows to fulfill the RGB channels. The interface circuit for the detection contains the scanning voltage generator, so, current detection requires a minimum of external components enabling it to be directly monitored near to the sensor, thus reducing the interferences and offering a compact design. Devices having different front and back i-layer thickness are analyzed under different voltage scan waveform to detect the RGB threshold voltages, and under different optical bias conditions to fulfill the RGB channels. As optical images it is used the light from a monochromator, in the 400 nm to 800 nm range, which corresponds to single wavelengths and the optical image from a printed rainbow mask, where the colors result from multiple wavelength combinations. Results show that in the single wavelength mode the threshold voltage between green and red sensitivity depends on the thickness of the bottom a-Si:H (-i) layer while between blue and green it depends on the front a-SiC:H (i)-layer thickness. As the thickness of the a-Si:H i-layer increases, the self-reverse effect due to the front absorption is balanced by the decrease of the self-forward effect due to the back absorption shifting the threshold voltage to lower reverse bias. In the multiple wavelength combinations mode, the output signal will be the weighted balance of the composing ink wavelength. In this mode, the gamma correction technique is used to

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compensate, the reverse or the forward self voltage effects in the bottom diode, respectively, due to the front or back confinement of the blue or red components of the subtractive printer system. The various design parameters and image reconstruction algorithms are discussed. A physical model supported by electrical and numerical simulations give insight into the methodology used for image representation and color discrimination.

PHOTOCURRENT AND SPECTRAL RESPONSE ANALYSIS OF A-SIC:H PINIP AND PINPIN PHOTODIODES

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

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

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OPTICAL MULTIPLEXER FOR SHORT RANGE COMMUNICATIONS

Louro, P.[1,2]; Vieira, M.[1,2]; Vieira, M.A.[1,3]; Fernandes, M.[1]; Fantoni, A.[1]; Francisco, C.[1]; Barata, M.[1,2]

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Livros de Resumos da European Research Spring Meeting, Simpósio C: Frontiers in silicon-based photonics, Estrasburgo, França, 26 a 30 de Maio de 2008.

A multiplexer is a device that combines two or more signals onto a single output. This is a useful tool for the transmission of signals that can share the same physical transmission path. At the end of the connection it is necessary to have a demultiplexer that performs the inverse operation, and allows the recovery of each input signal. In this paper we present results on the use of multilayered a-SiC:H heterostructures as wavelength-division multiplexing device (WDM) operating in the visible region of the electromagnetic spectrum. The WDM is a glass/ITO/a-SiC:H (p-i-n)/ a-SiC:H(-p) /Si:H(-i)/SiC:H (-n)/ITO heterostructure in which the generated photocurrent at different values of the applied bias can be assigned to the different optical signals. The device was characterized through spectral response measurements, under different electrical bias and frequencies. Results show that in the multiplexing mode the output signal is balanced by the wavelength of each incoming optical carrier and modulated by their frequencies. An analysis based on a theoretical model, a SPICE simulation of an equivalent electrical model and a numerical ASCA simulation are executed for describing the behavior of different configurations of the device and compared with experimental measurement about spectral response and current-tension characteristic. Finally it is presented a conclusion about the applicability of these devices in large area electronic applications.

LARGE AREA A-SIC:H WDM DEVICES FOR SIGNAL MULTIPLEXING AND DEMULTIPLEXING IN THE VISIBLE SPECTRUM

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Results on the use of a double a-SiC:H p-i-n heterostructure for signal multiplexing and demultiplexing applications in the visible range, are presented. The absorption coefficient of the front photodiode 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 range. Modulated monochromatic beams together (multiplexing mode), or a single polychromatic beam (demultiplexing mode) impinge in the device and are absorbed, accordingly to their wavelength, giving rise to a time and wavelength dependent electrical field modulation across it.
Dual wavelengths combinations using red, green and blue pulsed input channels are transmitted together, each one with a specific transmission rate. The combined optical signal is analyzed by reading out, under different applied voltages, the generated photocurrent. Results show that in the multiplexing mode the output signal is balanced by the wavelength and transmission rate of each input channel, keeping the memory of the incoming optical carriers. In the demultiplexing mode the photocurrent is controlled by the applied voltage allowing regaining the transmitted information. An electrical model gives insight into the device operation.

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VOLTAGE CONTROLLED WDM DEVICES IN THE VISIBLE SPECTRUM: A SPICE SIMULATION

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Livros de Resumos da 6th IBERSENSOR VI Congresso Ibero-americano de Sensores, São Paulo, Brasil, 24 a 26 de Novembro de 2008.

A multiplexer is a device that combines two or more signals onto a single output without losing their specificity. This paper presents results on the applicability of a multilayered a-SiC:H heterostructures as an electrically programmable optical filters for WDM transmission over POF. An electrical model supported by a SPICE simulation is presented to give inside the WDM device operation. The WDM is a double pin a-SiC:H heterostructure which faces the modulated light incoming together from different beams, each one with a specific wavelength and transmission rate. The spectral sensibility of the device is voltage controlled allowing the recovering of the input channels. Results show that the output signal has a strong nonlinear dependence on the light absorption profile, i.e. on the incident light wavelength, frequency and intensity due to a self biasing of the junctions under certain unbalanced light generation of carriers. By switching between positive and negative voltages the input channels can be recovered or removed. So, this optical device allows to add and drop one or several channels (OADMS) in a WDM optical network and can be used in optical communications.

OPTICAL WAVELENGTH-DIVISION MULTIPLEXING/DEMULTIPLEXING DEVICES

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Results on the use of a double a-SiC:H p-i-n heterostructure for signal multiplexing and demultiplexing applications in the visible range, are presented. Pulsed monochromatic beams together (multiplexing mode), or a single polychromatic beam (demultiplexing mode) impinge in the device and are absorbed, accordingly to their wavelength. Red, green and blue pulsed input channels are transmitted together, each one with a specific transmission rate. The combined optical signal is analyzed by reading out, under different applied voltages, the generated photocurrent. Results show that in the multiplexing mode the output signal is balanced by the wavelength and transmission rate of each input channel, keeping the memory of the incoming optical carriers. In the demultiplexing mode the photocurrent is controlled by the applied voltage allowing regaining the transmitted information. An electrical model gives insight into the device operation.

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Livros de Resumos da 6th IBERSENSOR VI Congresso Ibero-americano de Sensores, São Paulo, Brasil, 24 a 26 de Novembro de 2008.

ANÁLISE E COMPARAÇÃO DE ALGORITMOS DE CÁLCULO DE POSIÇÕES GPS

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Publicado em:
Actas da JETC'08 IV Jornadas de Engenharia Electrónica e Telecomunicações e de Computadores, Lisboa, Novembro de 2008, pp. 302-307.

A presente proposta visa a determinação e apresentação dos tempos associados ao processamento de algoritmos de cálculo de posicionamento GPS, por referência a uma coordenada conhecida, nos vários modelos de Terra (esférica, plana e elíptica) em diversas arquitecturas. Para tal serão testadas e comparadas diversas arquitecturas de 8 e 32 bits, de âmbito genérico e para sistemas dedicados.

COMPLETE DISTRIBUTED GARBAGE COLLECTION FOR .NET REMOTING

Barros Pereira, Paulo Alexandre Leal

Mestrado em: Conectividade e Sistemas Distribuídos
Grau Concedido por: Instituto Superior Técnico
Orientadores: Paulo Ferreira e Luís Veiga
Provas Concluídas em: 2 de Junho de 2008

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, while maximizing application programmers' productivity, requires automatic memory management, named distributed garbage collection (DGC).
We propose a novel taxonomy for DGC algorithms' classification. The taxonomy emphasizes distributed garbage identification techniques, since actual reclamation is assumed to be performed by existing local garbage collectors. To assess it, a survey of DGC algorithms is presented. Algorithms' outlines and analysis are grouped according to their classification in this taxonomy and are made considering distribution issues, such as coordination requirements, locality of action, communications network usage, and fault tolerance.
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 distributed garbage collectors either run on specialized environments or require modifications of the underlying virtual machine, hindering its immediate utilization.
This document describes the design and implementation of a DGC service for .NET Remoting (.NET's distributed object system) that: i) is capable of reclaiming both *acyclic* and *cyclic garbage*, while ii) being portable in the sense that it does not require modification of the underlying virtual machine, making use of the provided aspect-oriented functionalities. The obtained performance results are encouraging.

IDENTIFICAÇÃO DAS INTERACÇÕES DE SERVIÇOS PERSONALIZADOS

Sousa Leite, Nuno Miguel da Costa de

Mestrado em: Engenharia Electrotécnica e de Computadores
Grau Concedido por: Instituto Superior Técnico
Orientadores: Rui Gustavo Nunes Pereira Crespo
Provas Concluídas em: 20 de Maio de 2008

A crescente utilização da Internet motivou o desenvolvimento dos serviços oferecidos em aplicações como correio electrónico ("Email"), telefonia sobre a Internet ("VoIP") e WWW. A integração de novos serviços levou à inevitável ocorrência de interacções, com comportamentos indesejáveis.
Nesta dissertação analisa-se o problema da detecção das interacções de serviços na Internet. Propõe-se a extensão dos métodos existentes com vista a suportar a detecção de interacções de serviços com personalização. O tipo de interacções indesejadas a detectar inclui as interacções entre pares de serviços subscritos por um único utilizador numa máquina.
Descreve-se a arquitectura e implementação de um simulador que realiza a detecção de interacções dos serviços subscritos por um utilizador. A aplicação desenvolvida permite realizar a especificação de serviços e personalizações de forma simplificada, através de uma interface gráfica.
Estabelece-se um modelo usando lógica de predicados e Prolog para representar os serviços e personalizações sendo a detecção de interacções realizada por identificação de incoerências das fórmulas lógicas. A identificação de incoerências auxilia o utilizador na escolha dos serviços a subscrever, evitando interacções.
A arquitectura do simulador assenta em tecnologia Java e teve como critérios de desenho: a riqueza funcional e facilidade de uso; o desempenho e a portabilidade.
Os resultados obtidos demonstraram o funcionamento da solução de acordo com os objectivos do projecto.

INFINITESIMAL AND COMBINATORIAL RIGIDITY APPROACHES FOR COARSE-GRAINING

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Doutoramento em: Biofísica
Grau Concedido por: Imperial College, London, UK
Orientadores: M. Barahona, S. Yalirak
Provas Concluídas em: Junho de 2008

O objectivo principal desta tese de doutoramento consiste em desenvolver e optimizar sensores de imagem e de cor com leitura e endereçamento ópticos.
Infinitesimal and Combinatorial Rigidity for Coarse-Graining The main goal of this work was to develop a software framework for the simulation of the dynamical, structural and electronic properties of nanosystems that can be represented by a network of constraints. Building upon the mean field theory or Maxwell Constraint Counting an exact algorithm for selecting the degrees of freedom based on the sparsity of the Rigidity Matrix was presented. A very efficient non-exact rigidity algorithm was also presented which scales linearly with the size of the system.
A molecular dynamics coarse-grained model based on constraint theory was implemented which can be applied to study the dynamical and rigidity properties of several constrained systems, including amorphous materials and small peptides in solution.

03

ENGENHARIA MECÂNICA

Anuário Científico 2008

ISEL

ELECTRODEPOSITION AND CHARACTERIZATION OF POLYPYRROLE FILMS ON ALUMINIUM ALLOY 6061-T6

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Polypyrrole films on aluminium alloy 6061-T6 were prepared by electropolymerization of pyrrole in sulphuric acid using two different processes – cyclic voltammetry and potentiostatic polarization – and assessed through SEM observation and voltammetry. The anticorrosive properties of these films were studied by polarization curves and electrochemical impedance spectroscopy. The polypyrrole films formed by both methods are homogeneous and present a globular structure. However, it was found that the films produced by cyclic voltammetry are thicker than those produced potentiostatically at a potential equal to the upper limit of the cyclic voltammetry (Eλa). It was also found that there is an optimum value for the formation potential (Eappl, in the case of the potentiostatic method or Eλa for cyclic voltammetry). Above this value, overoxidation of the polymer occurs, which is found to be deleterious to the coated system behaviour. From polarization curves no major differences were detected between the PPy-coated alloy and the bare material, indicating that no significant protection is achieved by the polymer coating. On the other hand, Bode diagrams are typical of a system undergoing pitting corrosion and show lower impedance values for the alloy covered with polypyrrole than for the bare metal. This can be attributed to the conductive character of the polypyrrole films.

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Electrochimica Acta, 2008, 53, 4754-4763.

03

IDENTIFICATION AND CONTROL OF THE AWS USING NEURAL NETWORKS MODELS

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Publicado em:
Applied Ocean Research Journal, 2008, 30, 178-188.

The Archimedes Wave Swing (AWS) is a fully-submerged Wave Energy Converter (WEC), that is to say, a device that converts the energy of sea waves into electricity. A first prototype of the AWS has already been built and tested. In this paper, neural network (NN) models for this AWS prototype are developed. NNs are then used together with proven control strategies (phase and amplitude control, internal model control and switching control) to maximise energy production. Simulations show an yearly average electricity production increase of 160% over the performance of the original AWS controller.

I-MERC: UM NOVO CONCEITO PARA A SEGURANÇA E QUALIDADE DA DISTRIBUIÇÃO DE REFEIÇÕES

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O transporte de refeições nos serviços de saúde em condições de segurança e a transmissão eficiente de informações acerca das dietas personalizadas dos doentes são um desafio diário para todos os intervenientes no processo. A contaminação bacteriológica das refeições e da cozinha, os métodos utilizados para identificação das refeições demasiado arcaicos e ineficientes e a dificuldade em manipular os veículos quando estão carregados são os maiores problemas sentidos nos serviços de logística alimentar.
Para melhorar a qualidade dos serviços de entrega de refeições nos serviços de saúde, propõe-se um transportador automático – o i-Merc – desenvolvido em duas versões, autónoma e servo-assistida, com compartimentos pré-aquecidos, um sistema de controlo da temperatura das refeições e um sistema de gestão de refeições integrado.
Na versão autónoma, o transporte é realizado por um robô móvel garantindo uma ausência de esforço físico e mobilidade de pessoas entre cozinha e enfermaria, enquanto o servo-assistido é mais económico e fácil de implementar nos serviços de saúde existentes.

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Revista Robótica, 2008, 72 (3º trimestre), 4-10.

03

AN APPROACH TO DYNAMIC MAINTENANCE BASED ON ACTUAL DATA

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Publicado em:
Actas do 34th ESReDA Seminar – Supporting Technologies for Advanced Maintenance Information Management, San Sebastian, Spain, 13 e 14 de Maio de 2008, Lecture nº 5, 16 pág..

Maintenance plays a very important role in almost industrial activities. As there is a great concern about equipment availability and people and environment safety all over the world, that makes maintenance the central operational function of most industrial activities above all in those that are capital intensive and/or where there are high safety risks. So, decisions about the correct methods to apply to maintenance, the best techniques to use and the equipment failure forecast depend more and more on the technological quality of the maintenance activities deployed. These ones depend on the capacity to gather and treat reliable data and information about equipments condition. The efficiency of organization strategies as TPM or RCM can only be achieved if they are based in correct data and information analysis.

If it can be predicted a failure by monitoring a critical operational parameter characteristic of the equipment and if this prediction allows to plan a preventive maintenance activity on the equipment at the correct time (not too early, not too late), it is possible to take advantage of a better equipment availability for production, acting for maintenance activities only when necessary and without the concerns and consequences of failure occurrences.

Actual equipment data can be collected and gathered by the use of appropriate sensors, by equipment performance measurements or by any other possible techniques that are able to reveal the real condition of equipment relative to its degradation. In accordance with the measured values, it is possible to sketch tendency curves dependent on relevant parameters and then it can be made a calculation of the time to failure, assuming there is a failure when a monitored parameter reaches a critical value.

This methodology can be applied to critical process systems and equipments, where failures may have a high economical and/or safety impact. It can be applied instead of the more traditional approaches to maintenance, as are systematic or corrective maintenance, or as a complement of those approaches.

This paper outlines the importance of testing, inspection and mainte-

nance operations. It is proposed a methodology based on real operational data from the measurement of selected equipment parameters (vibration, temperature,...) analysis and its evolution with time, to support maintenance actions, according to the actual degradation condition of components. Also, in this paper it is shown the importance of the gathering and treatment of real data using modern monitoring technologies, combining reliability analysis with fuzzy logic and in a dynamic way to allocate maintenance actions on time.

ANÁLISE FIABILISTICA DE SISTEMAS DE SEGURANÇA – DO CONCEITO À PRÁTICA

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Actas do 6º Simpósio Internacional de Confiabilidade, Florianopolis, Brasil, 7, 8 e 9 de Maio de 2008, pp. 381-396.

Este trabalho tem como finalidade desenvolver uma metodologia destinada a uma análise funcional e análise de risco de um equipamento pertencente a um sistema de extinção de incêndio. Este sistema está normalmente inserido no projecto de segurança e prevenção de incêndio, complementando outros sistemas, tais como a detecção de incêndio e desenfumagem, contribuindo para a redução ou inexistência das possíveis consequências em caso de ocorrência de um evento desta natureza.
Alguns edifícios, quer pelas suas características construtivas, quer pela diversidade dos produtos que contêm ou pela alta taxa de ocupação que normalmente verificam, justificam à partida uma análise cuidada da fiabilidade e disponibilidade dos equipamentos de combate a incêndio.
As Centrais de Bombagem de uma Rede de Incêndios são equipamentos de combate a incêndio que normalmente são alvo de um projecto e instalação correctos, mas, infelizmente, após a entrega aos proprietários do edifício são esquecidos, deixando de lado questões fundamentais como a segurança das pessoas e bens e comprometendo o seu bom funcionamento quando realmente é necessário.
Com base nesta preocupação foi elaborado um estudo aplicado a uma instalação específica – a Estação do Oriente, situada no Parque das Nações em Lisboa. Este estudo é centralizado na análise funcional dos equipamentos e tem por base uma Análise de Modos de Falha e Efeitos (FMEA).
O trabalho desenvolvido permite uma posterior aplicação a qualquer sistema, e mostra as dificuldades sentidas pelos profissionais nas questões relacionadas com a Fiabilidade.

AUTONOMOUS DRIVING COMPETITION: TEACHING CONTROL CONCEPTS IN A VIRTUAL REALITY ENVIRONMENT

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This paper describes a Virtual Reality application that reproduces the environment of the Autonomous Driving Competition and suggests that this application constitutes an adequate platform for assigning engaging exercises and addressing fundamental issues in Control Engineering and Computer Science courses. Even though our approach eliminates the benefits of practical experience that can only be acquired with direct contact with real robots, we believe that additional benefits make it valuable. Firstly, the VR media is intrinsically attractive and provides intuition that usually is not achieved through classic simulations. Secondly, the VR application can be easily accessed and programmed by the students, contrarily to the "hardware" version of the problem, which requires access to a fully equipped mobile robot and a room with a set up similar to the one used in the robot competitions. Thirdly, if the school assigning these exercises does possess mobile robots fit for competition, these exercises can be regarded as a test bed for developing control strategies that will be, in a later stage, tried by the student on the real robot. As an example, we show that touching only a few challenges that arise from the competitions specifications lead us to the exploration of the problem of mobile robot control and to the study of methods in Fuzzy Systems, Artificial Vision and Neural Networks.

Publicado em:
Actas da 8th Portuguese Conference on Automatic Control, Vila Real, Portugal, 21 a 23 de Julho de 2008, pp. 308-314.

COMPARISON OF CONTROL STRATEGIES PERFORMANCE FOR A WAVE ENERGY CONVERTER

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Proceedings of the 16th Mediterranean Conference on Control and Automation, Ajaccio, France, 25 a 27 de Junho de 2008, pp. 773-778.

The Archimedes Wave Swing (AWS) is a a fully submerged Wave Energy Converter (WEC), that is to say, a device that converts the kinetic energy of sea waves into electricity. A first prototype of the AWS has already been built and tested. This paper presents simulation results of the performance of several control strategies applied to this device, including PID control, reactive control, phase and amplitude control, latching control, feedback linearisation control, internal model control, switching control, and combinations thereof. Linear, white-box nonlinear, and neural network models were employed. Significant (above threefold) increases in yearly energy production were found to be possible with properly designed control strategies.

COMPORTAMENTO ELECTROQUÍMICO DA LIGA DE NITI

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O comportamento electroquímico da liga NiTi foi avaliado em soluções fisiológicas a 37ºC e para diferentes valores de pH a fim de simular as condições "in vivo". Para efeitos comparativos ligas usualmente utilizada como biomateriais (Ti-6Al-4V e aço inoxidável 316L) foram também estudadas. De modo a compreender o efeito dos elementos de liga no comportamento do Nitinol, incluiu-se neste trabalho titânio e níquel puros. Este estudo permitiu concluir que a resistência à corrosão do Nitinol é semelhante à da liga Ti-6Al-4V e superior ao aço 316L uma vez que este, nas mesmas condições, é susceptível à corrosão por picadas. Concluiu-se também que o comportamento do Nitinol é independente do pH do meio agressivo na gama estudada (pH de 3 a 10). A análise da superfície da liga NiTi for realizada por XPS após polimento mecânico e após 3 dias de imersão na solução de Hank. Os espectros obtidos revelaram a presença dum filme de óxido, apresentando um quociente Ti:Ni ~ 95:5 para o caso da amostra imersa, indicando que o filme passivo é maioritariamente constituído por Ti(IV). Verificou-se também que a imersão na solução fisiológica conduz a um aumento da espessura do filme.

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Actas do 28º Congresso Brasileiro de Corrosão and 2nd International Corrosion Meeting (Intercorr 2008), Recife, Brasil 12 a 14 de Maio de 2008.

COMPUTATIONAL APPROACHES TO HUMAN ARM MOVEMENT CONTROL - A REVIEW

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Publicado em:
Actas do 17th IFAC World Congress, Seul, Coreia, 6 a 11 de Julho de 2008, pp. 15716-15723.

Human arm movement control theories are reviewed in the current paper. The motor planning problem stated as a generation of a time plan for the execution of a movement task, is a major concern of the current paper. It will be shown that computational models of motor control have a strong potential for the use in the area of human motor rehabilitation. Their use can be discriminated in three main areas of application: the generation of correct trajectories to be demonstrated to human subjects during physiotherapy; the assessment of motion disorders and movement quality; and the devising of challenging interaction exercises that promotes recovery. This paper will review the major theories pointed out for the purpose of describing human arm movement control. In particular, computational theories are presented, that is, mathematical models for motor control that can be simulated in a computer and compared against measured data. The aim of this paper is to extract knowledge from these theories that can be useful for the purpose of motor rehabilitation.

COMPUTER ASSISTED TECHNOLOGIES IN THE DEVELOPMENT OF PROTOTYPES

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In the industry computer assisted technologies are being implemented very fast. Most companies support the use of the new computer assisted technologies as a fully integrated digital policy. Currently, due to the high number of available alternatives in the market, the integration analysis of the computer assisted conception and production technologies is a critical study, in order to establish the potential for a full implementation of a CIM (Computer Integrated Manufacture) strategy.

The technology developments in the area of computer assisted project and production of prototypes is reviewed in this paper. The text is divided in five main topics, namely: i) an introduction to the characteristics of actual markets requirements and demands of clients that lead to the need of new methods and equipments to be used by the production companies, ii) a review about the available capabilities on computer assisted conception and production technologies (computer-aided design/engineering/manufacturing and rapid prototyping); iii) an analysis about product designer standards and requirements (an example concerning the making of working drawings is used to illustrate the actual constraints in the computer assisted technologies); and iv) conclusions regarding the state of the art and future developments preview in the area.

Publicado em:
Proceedings do World Congress on Engineering 2008 (WCE 2008) - International Conference of Manufacturing Engineering and Engineering Management, promovido pela International Association of Engineers, Londres, Inglaterra, 02 a 04 de Julho de 2008, pp. 1208-1213.

CONCEPTION AND MANUFACTURING OF ECO-MARATHON VEHICLE MECHANICAL SYSTEMS

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Publicado em:
Proceedings da 18th International Conference on Flexible Automation and Intelligent Manufacturing (FAIM-2008), Skovde, Suécia, 30 de Junho a 02 de Julho de 2008, pp. 237-244.

In this work are described the main phases of conception and construction of an ecological vehicle, made by students and teachers, whose objective is to participate in the Eco-marathon student contest. The objective of this contest is to spend the less fuel possible by kilometer run. To attain that, the weight, drag and performance of mechanical systems, were object of analysis. The aluminum chassis, FRP wheel's hubs and the power transmission system, that incorporates a magnetic clutch, were conceived by the team of students and teachers. The 3D modelation was made with SolidWorks and Inventor software. FEM analysis was performed in CosmosWorks, Ansys and Cosmos Motion. Some prototypes are being produced, by means of a four-axis CNC vertical machining center. The CAM programming was made using CATIA V5 CAM module. Design for manufacturing is taken into account, and fabrication of these prototypes is being used to test the jig fixtures, in order to control the established accuracy and surface finishing of the parts. Methodologies that allow machining of the designed parts, according to their specified tolerances, based on the evaluation of different variables in the CAM system, were also investigated.

DIMENSION AND COVERAGE OF MULTIPLE-MODELS STRUCTURES USING CLUSTERING TECHNIQUES

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In this work a method for building multiple-model structures is presented. A clustering algorithm that uses data from the system is employed to define the architecture of the multiple-model, including the size of the region covered by each model, and the number of models. A heating ventilation and air conditioning system is used as a testbed of the proposed method. In this work the main objective was to design an algorithm that is able to overcome one of the most difficult tasks associated with the multiple-model approach: the selection of the operating regimes and the appropriate number of models to cover the space of input and output variables. The design was based on clustering techniques.

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DESIGN OF DISTRIBUTED FAULT TOLERANT CONTROL SYSTEMS

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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. Despite the research effort on developing FTC systems for NCS most of these developments still being designed globally leading to centralized FTC solutions inadequate to NCS or, assume the communication network and the process itself as two different entities loosing the potentiality of the integrated design. The FDI/FTC design method presented in this paper is able to use 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. The design methodology is made easy using a FTCNS-MAS toolbox introduced in this paper.

INHERENTLY CONDUCTING POLYMERS ON ALUMINIUM ALLOY 6061-T6 BY ELECTROPOLYMERIZATION

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Among ICP's investigated for corrosion protection, polypyrrole (PPy) and polyaniline (PANI) are the most studied and have been prepared by electropolymerization of pyrrole or aniline on inert electrodes such as gold and platinum and also on stainless steel or copper. However, it is much more difficult to generate these polymers on valve metals such as aluminum and aluminum alloys. This could be related with the formation, on the metal surface, of a thin, but highly stable protective oxide-hydroxide layer that blocks electron transfer and impedes polymer formation and deposition. Furthermore, this oxide usually grows at positive potentials in the acidic conditions normally required for the electrosynthesis of conducting polymers. In this work, some results concerning electrodeposition of polypyrrole and polyaniline on 6061 T6 aluminum alloy by two different processes (cyclic voltammetry and a potentiostatic method) will be presented. The coatings have been assessed through SEM observation and voltammetry and their anticorrosive properties were studied by polarization curves and electrochemical impedance spectroscopy.

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Actas do 17th International Corrosion Congress (ICC'08), Las Vegas, EUA, 4 a 10 de Outubro de 2008.

INTELLIGENT TRANSPORT SYSTEM BASED ON RFID AND MULTI-AGENT APPROACHES

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Actas do 9th IFIP Working Conference on Virtual Enterprises, 8 a 10 de Setembro de 2008, Poznan, Polónia, CD-ROM.

This paper presents an Intelligent Information and Communication Technology (IICT) architecture able to cope with the nowadays logistics operators challenges. The aim is to achieve an Intelligent Transport System based on RFID together with Multi-agent systems. Furthermore, the logistical platforms (production or distribution), as nodes of added value of supplying and distribution networks, are proposed as critical points of the visibility of the inventory, where these technological needs are more evident.

O ENSINO DE HIGIENE E SEGURANÇA INDUSTRIAL NUMA LICENCIATURA EM ENGENHARIA MECÂNICA – O CASO DO ISEL

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Publicado em:
Actas do Colóquio Internacional de Segurança e Higiene Ocupacionais 2008 (SHO 2008), Universidade do Minho, Guimarães, 7 e 8 de Fevereiro 2008, pp. 311-314.

A segurança constitui hoje em dia, tal como a qualidade, um factor de competitividade na indústria. Faz, necessária e inquestionavelmente, parte dos eixos estratégicos da gestão empresarial, a par e em igualdade, com áreas como a gestão financeira, a gestão dos recursos humanos ou a gestão da produção.

O engenheiro encontra-se, em todas as áreas da sua actuação profissional, confrontado e responsabilizado, tanto profissional com socialmente, com os custos e os efeitos da "não segurança".

A u.c. de Higiene e Segurança Industrial (HSI) foi criado no ISEL no ano lectivo de 1989/90, aquando da reestruturação curricular, pretendendo-se colmatar uma lacuna na formação de base, tanto técnica como de gestão, dos futuros engenheiros mecânicos.

Começa-se, nesta comunicação, por situar, justificando-a nos seus pressupostos e enquadramento enformadores da sua criação, a introdução - exemplar e precursora no contexto das escolas do ensino superior de engenharia em Portugal -, da disciplina de HSI no Departamento de Engenharia Mecânica (DEM).

Apresentam-se os objectivos e metodologia da disciplina (agora, unidade curricular no quadro pós-Bolonha) bem como os recursos utilizados na sua leccionação.

Detalha-se o programa e as opções subjacentes, explicitando-se as actividades complementares ao ensino e aprendizagem das matérias curriculares (em particular as *Conferências Temáticas sobre Segurança Industrial* e as *Palestras sobre Segurança e Saúde do Trabalho*, destinadas aos alunos de HSI mas abertas a todo o ISEL, como ao exterior, com a significativa presença tanto de técnicos da indústria e instituições), apresentando-se, ainda, os resultados da sua avaliação (inquéritos aos alunos, internos à disciplina).

Conclui-se pela constatação da consolidação desta u.c. no currículo das novas licenciaturas, não só pelos objectivos programáticos cabalmente alcançados (formação de base e competências adquiridas pelos alunos e, também, no despertar da consciência e apetência para matéria "parente pobre" da formação de base e da prática da engenharia), alicerces que permanecerão, constituindo semente útil que frutificará e amplificar-se-á na futura actividade profissional dos jovens engenheiros.

RISCO QUÍMICO: COMUNICAÇÃO DO PERIGO

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Publicado em:
Actas do Colóquio Internacional Segurança e Higiene Ocupacionais 2008 (SHO 2008), Universidade do Minho, Guimarães, 7 e 8 de Fevereiro 2008, pp. 315-319.

A comunicação do perigo respeitante às substâncias e preparações perigosas revela-se de importância crucial para todos os cidadãos, tanto enquanto consumidores como, no contexto da segurança industrial e/ou do trabalho, para os trabalhadores profissionalmente expostos.
Desde 1967 que a União Europeia tem vindo a desenvolver e a aplicar um sistema harmonizado de classificação, embalagem e rotulagem de substâncias e preparações perigosas.
O *Sistema Mundial de Classificação e Rotulagem de Substâncias Químicas (GHS)* foi adoptado pelo Comité Económico e Social da Organização das Nações Unidas em 2005, estabelecendo princípios e critérios coerentes, globalmente harmonizados e aceites visando uma protecção mais transparente, universal e eficaz.
No âmbito específico da comunicação do perigo, partindo do actual sistema comunitário sobre classificação, rotulagem e embalagem de substâncias perigosas, enquadrado no novo sistema REACH - registo, avaliação, autorização e restrição de substâncias químicas -, faz-se, nesta comunicação, a apresentação da recente proposta da Comissão Europeia para um novo regulamento comunitário que visa incorporar o GHS no *aquis* da União Europeia (Regulamento CRE).
Faz-se a revisão dos seus vectores fundamentais situando e explicitando, em conjunção com o RID/ADR (Regulamentação do transporte internacional de mercadorias perigosas por estrada) ao qual o GHS se encontra indissociavelmente ligado por via da sua génese, os seus pressupostos, objectivos e conteúdo, realçando-se as alterações tanto no respeitante às fichas de dados de segurança como, e sobretudo, á nova rotulagem (novos pictogramas de perigo, palavras-sinal, advertências e recomendações de perigo,...), elementos fundamentais na gestão da segurança industrial e do trabalho no respeitante à exposição profissional a gentes químicos perigosos.

ROLLING BEARING FAULT DETECTION AND ISOLATION - A DIDACTIC STUDY

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The present paper aims to demonstrate why usually when theoretical mathematical models are used to compute the frequencies corresponding to a faulty rolling bearing a deviation is obtained between the computed values and the real frequencies emitted by such a device. A lab rolling bearing test ring has been developed to perform the current studies.

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Actas da 4th WSEAS/IASME International Conference on EDUCATIONAL TECHNOLOGIES (EDUTE'08), Corfu, Grécia, 26 a 28 de Outubro de 2008, pp. 132-137.

SENTIENT OBJECTS FOR DESIGNING AND CONTROLLING SERVICE ROBOTS

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Services related to healthcare and the support for elderly people become more and more important. Autonomous or semi-autonomous robots may play an important role in this area. From a control system point of view these robots are networks of distributed smart components to perceive their environment and react on it in real time. The problem of developing or extending such a robot often is that the designer has to start from scratch struggling with low level issues, where reusability of already designed components would be highly desirable. The paper describes a robot application in the area of a meals distribution service that combines two design worlds. One is the conventional world of modeling the functional properties without any structural considerations, the other is the world of cooperating sentient objects. We explain how the notion of sentient objects will assist the design, simulation and also later extensions and adaptations of the robot.

SWITCHING CONTROL OF THE ARCHIMEDES WAVE SWING

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Control switching is applied to the Archimedes Wave Swing (AWS), a device designed to convert the energy of sea waves into electricity. Previous simulations showed that energy production can be significantly increased using Internal Model Control, together with direct and inverse Elman Neural Network (NN) models of the AWS, and a reference based
upon the phase and amplitude control strategy. Since the best performance was achieved by different NN models depending on the month of the year, further simulations were carried out showing that switching between different controllers, corresponding to different models, according to the spectrum of the incoming wave, further increases energy production.

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03

AVALIAÇÃO DE DESEMPENHO DOS PRINCIPAIS TERMINAIS DE CONTENTORES DA PENÍNSULA IBÉRICA

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Publicado em:
Livros de Resumos do XI Jornadas Técnicas, O Sector Marítimo Português, CENTEC (Centre for Marine Technology), Instituto Superior Técnico, IST, 25 a 27 de Novembro de 2008.

A eficiência das operações de um terminal intermodal de carga contentorizada tem sido objecto de estudo de vários investigadores. O método mais objectivo para quantificar os indicadores chave de performance é o DEA (*Data Envelopment Analisys*).

Actualmente, este método utilizado em conjunto com a mineração de dados (Data Mining) traduz-se numa ferramenta de diagnóstico mais fiável na comparação dos dados operacionais dos portos. Este estudo aplicará esta metodologia para avaliar o desempenho portuário nos terminais de carga contentorizada no chamado *hinterland* ibérico desde o ano 2003.

Os indicadores de desempenho analisados são os tradicionalmente utilizados noutros estudos, acrescidos de alguns outros menos aplicados até então, mas que contribuem para uma descrição operacional detalhada dos portos em análise, e realçam os aspectos a melhorar ao nivel da gestão portuária. Em suma, considerando que os portos são nós das redes logísticas globais (ou interfaces de valor acrescentado cuja impedância ou somatório dos custos friccionais, em qualquer dos casos deve ser mínima), a avaliação referente ao seu desempenho é essencial para que se possam tomar decisões eficazes no sentido de aumentar a sua eficiência, a sua produtividade e, logo, a sua competitividade.

CORROSION BEHAVIOUR OF NITI MODIFIED BY THERMAL TREATMENT AT THE SURFACE

Figueira, N.[1]; Montemor, M.F.[1]; Silva, T.M.[1,2]; Carmezim, M.J.[1,3]; Fernandes, J.C.S.[1]

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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 their biocompatibility. However, due to the high nickel content of the alloy and as this element may induce allergic response, the material must present superior corrosion resistance in contact with body fluids.
The main objective of this work is developing and selecting NiTi surface modification treatments that may reduce surface degradation by corrosion, and, at the same time, guarantee a low nickel content on the surface.
In the present work, the electrochemical behaviour of NiTi has been studied in Hank's solution at 37ºC to simulate body conditions, before and after surface modifications.
An equivalent circuit was proposed to fit the impedance spectra of NiTi and electrochemical parameters were estimated to characterize its natural and modified passive oxide films.
XPS analysis established that both oxidized Ti and Ni can be found on the surface of polished NiTi alloy but after surface modification, a lower content of Ni is found.

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Livros de Resumos do XV Encontro da Sociedade Portuguesa de Electroquímica, Lisboa 3 a 6 de Setembro de 2008.

ELECTRODEPOSIÇÃO DE POLÍMEROS CONDUTORES NA LIGA DE ALUMÍNIO 6061-T6

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Livros de Resumos do 5º Congresso Luso-Moçambicano de Engenharia (CLME 2008), Maputo, Moçambique 2 a 4 de Setembro de 2008.

Ao longo da segunda metade do século XX o alumínio e as suas ligas impuseram-se como materiais de eleição em inúmeras aplicações, como, por exemplo, no caso da indústria automóvel ou da indústria aeronáutica. Para tal contribuíram as melhorias significativas das propriedades mecânicas do alumínio que foram conseguidas através da adição de elementos de liga como o cobre, o zinco ou o magnésio. Contudo, os precipitados formados por adição destes elementos, a par de aumentarem a resistência do material, provocam uma severa degradação da sua resistência à corrosão. Desta forma, o uso destes materiais apenas se torna viável se associados a sistemas eficazes de protecção anticorrosiva e, em particular, à aplicação de revestimentos adequados. Antes da pintura ou utilização de adesivos é normalmente necessária a utilização de pré-tratamentos. No entanto, os pré-tratamentos tradicionalmente usados para o alumínio e as suas ligas baseiam-se em cromatos, reconhecidos como compostos altamente tóxicos, cancerígenos e considerados perigosos do ponto de vista ambiental.

Nas últimas décadas, os polímeros condutores têm sido alvo de grande atenção como possíveis componentes de revestimentos anticorrosivos alternativos aos tratamentos baseados em cromatos [DeBerry 1985, Tallman 2002, Huerta-Vilca 2005]. Estes polímeros podem depositar-se nos metais a revestir por electropolimerização a partir de uma solução electrolítica contendo o monómero respectivo. Entre os monómeros que dão origem a polímeros condutores, a anilina e o pirrole têm sido os mais estudados.

O presente trabalho apresenta a produção de filmes de polianilina e polipirrole na liga de alumínio 6061-T6, através da electropolimerização dos respectivos monómeros (0,5 M) num electrólito suporte 0,5 M H_2SO_4, e a investigação do seu comportamento electroquímico. A electrodeposição foi efectuada usando voltametria cíclica e métodos potenciostáticos. A actividade electroquímica e as propriedades de protecção contra a corrosão dos filmes foram estudadas através de curvas de polarização, espectroscopia de impedância electroquímica e voltametria cíclica. A morfologia dos filmes foi investigada usando a técnica de microscopia electrónica de varrimento (SEM).

ESTUDOS DE CORROSÃO EM LIGAS DE NITINOL

Figueira, N.[1]; Silva, T.M.[1,2]; Carmezim, M.J.[1,3]; Fernandes, J.C.S.[1]

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Livros de Resumos das 5as Jornadas da Revista Corrosão e Protecção de Materiais, Lisboa, 20 de Novembro de 2008.

Nitinol é a uma liga de composição aproximadamente equiatómica de níquel e titânio, caracterizada por uma combinação única de propriedades, onde se incluem a superelasticidade e o efeito de memória de forma, o que a torna muito atractiva em aplicações biomédicas. No entanto, o alto teor em níquel desta liga pode provocar consequências nefastas em termos da sua biocompatibilidade. De facto, o níquel pode conduzir a efeitos alérgicos, tóxicos ou mesmo carcinogénicos. Por outro lado, foram encontrados na literatura diferentes pontos de vista em relação à resistência à corrosão do Nitinol e, consequentemente, à libertação de iões Ni.

No presente trabalho, foi estudado o comportamento electroquímico do Nitinol em soluções fisiológicas a 37ºC, de modo a simular as condições "in vivo". O mesmo estudo foi realizado com ligas habitualmente utilizadas para fins biomédicos, Ti-6Al-4V e aço inoxidável 316L, a fim de permitir realizar uma comparação, bem como com os elementos de liga Ti e Ni puros, de modo a entender a contribuição de cada um na liga, por recurso a técnicas electroquímicas e de análise de superfície.

Observou-se para a liga de Nitinol, um comportamento semelhante ao do titânio e, quando comparado com os restantes materiais utilizados no estudo, estabeleceu-se a seguinte relação em termos de resistência à corrosão: Aço inoxidável 316L ‹ NiTi ‹ Ti-6Al-4V.

A partir dos resultados acima obtidos foram idealizadas algumas formas de modificação da superfície do NiTi, de forma a reduzir os riscos de libertação de Ni para o ambiente fisiológico. Os detalhes destes ensaios de modificação e os respectivos resultados serão discutidos neste trabalho.

LIGA DE NITINOL PARA APLICAÇÕES BIOMÉDICAS: ESTUDOS DE CORROSÃO E MODIFICAÇAO DE SUPERFÍCIES

Figueira, N.[1]; Silva, T.M.[1,2]; Carmezim, M.J.[1,3]; Fernandes, J.C.S.[1]

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Livros de Resumos do 5º Congresso Luso-Moçambicano de Engenharia (CLME 2008), Maputo, Moçambique 2 a 4 de Setembro de 2008.

Nitinol é a uma liga de composição aproximadamente equiatómica de níquel e titânio, caracterizada por uma combinação única de propriedades, onde se incluem a superelasticidade e o efeito de memória de forma [Duerig, 1999], o que a torna muito atractiva em aplicações biomédicas. No entanto, o alto teor em níquel desta liga pode provocar consequências nefastas em termos da sua biocompatibilidade. De facto, o níquel pode conduzir a efeitos alérgicos, tóxicos ou mesmo carcinogénicos. Com efeito, foram encontrados na literatura diferentes pontos de vista em relação à resistência à corrosão do Nitinol e, consequentemente, à libertação de iões Ni [Shabalovskaya, 2002]. No presente trabalho, foi estudado o comportamento electroquímico do Nitinol em soluções fisiológicas, a 37°C, e a diferentes valores de pH de solução, de modo a simular as condições "in vivo". O mesmo estudo foi realizado com ligas habitualmente utilizadas para fins biomédicos, Ti-6Al-4V e aço inoxidável 316L, a fim de permitir realizar uma comparação, bem como com os elementos de liga Ti e Ni puros, de modo a entender a contribuição de cada um na liga, por recurso a técnicas electroquímicas e de análise de superfície. Foi anda testado o potencial de circuito aberto ao longo de uma gama de temperaturas. Observou-se para a liga de Nitinol, um comportamento semelhante ao do titânio e, quando comparado com os restantes materiais utilizados no estudo, estabeleceu-se a seguinte relação em termos de resistência à corrosão: Aço inoxidável 316L ‹ NiTi ‹ Ti-6Al-4V. O comportamento da liga de NiTi quando submetida a soluções com vários valores de pH levou a concluir que, em toda a gama de pH's estudados, esta manteve um comportamento típico de material passivo. A partir dos resultados acima obtidos foram idealizadas algumas formas de modificação da superfície do NiTi, de forma a reduzir os riscos de libertação de Ni para o ambiente fisiológico. Verificou-se que os tratamentos superficiais realizados sobre a superfície da liga aumentaram a resistência à corrosão e induziram uma diminuição no teor em Ni à superfície.

PORTUGAL E AS AUTO-ESTRADAS DO MAR; OPORTUNIDADES DE DESENVOLVIMENTO TECNOLÓGICO

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Esta apresentação propõe uma participação nacional inovadora no projecto europeu "Auto-Estradas Marítimas" que, na sua essência, assenta em premissas de ordem tecnológica. Conclui-se que Portugal, através deste projecto, não será muito beneficiado em termos do acréscimo da movimentação portuária e do transporte marítimo. Por isso, a vantagem competitiva nacional deve basear-se na liderança de projectos de investigação e inovação através das universidades, empresas e dos recursos humanos qualificados disponíveis. Devem aprofundar-se as Tecnologias da Informação e Comunicação Inteligente e o *RFID* com a utilização de Sistemas Multi-Agente, enquanto amortecedores da complexidade do funcionamento em rede das cadeias de valor, bem como suporte aos movimentos colaborativos emergentes nas redes logísticas. Finalmente, este artigo propõe a utilização de plataformas logísticas como centros de racionalidade das plataformas tecnológicas a partir das quais os sistemas de transportes e os portos envolvidos devem ganhar eficiência, de maneira a assumir o desafio das Auto-Estradas Marítimas como nova fonte de vantagem competitiva.

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SURFACE MODIFICATION OF NITINOL: AN ELECTROCHEMICAL STUDY UNDER SIMULATED PHYSIOLOGICAL CONDITIONS

Figueira, N.[1]; Carmezim, M.J.[1,3]; Silva, T.M.[1,2]; Fernandes, J.C.S.[1]; Ferreira, M.G.S.[1]

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Nitinol is a near-equiatomic alloy that presents shape memory effect and high elastic deformation. These properties, along with high fatigue strength, corrosion resistance and superior biocompatibility, have resulted in several applications as medical device material. A current problem with Nitinol implant devices is the release of nickel into the human body which can lead to inflammatory and allergic processes. In order to overcame this handicap a great effort has been done on Nitinol surface modifications and coatings research.
In this work the electrochemical behaviour of surface modified Nitinol (by thermal and chemical treatments) have been investigated in simulated physiological conditions (Hank's solution at 37°C) and compared with untreated Nitinol. These studies were carried out by electrochemical impedance spectroscopy, capacitance and photocurrent measurements and the resulting surfaces were characterised by Auger spectroscopy and XPS as well as by atomic force microscopy (AFM).
The doping densities (N_D) and the flatband potentials (U_{FB}) of the oxide films were determined using the Mott-Schottky approach. The films reveal n-type semiconductor behaviour. According to capacitance results, the oxide films formed by thermal oxidation present lower capacitance and higher donor density when compared with untreated Nitinol. The passive films show photocurrent response with optical band gaps ranging from 3.0 to 3.3 eV, which are in agreement with the value of 3.2 eV attributed to pure titanium oxide. For films formed by thermal oxidation and by chemical treatment the surface analysis data revealed a significant dependence of the Ni/Ti ratio on the type of treatment and temperature. The topography of films surfaces - in the nano-domain - and crystalline degree - was evaluated by AFM.

TRIBOCORROSION ASSESSMENT OF NiTi IN PHYSIOLOGICAL ELECTROLYTE: A PRELIMINARY STUDY

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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 their biocompatibility. However, due to the high nickel content of the alloy and as this element may induce allergic response, the material must present superior corrosion resistance in contact with body fluids. The authors of the present work are currently involved in a project with the main objective of developing and selecting NiTi surface modification treatments that may reduce surface degradation by corrosion and wear-corrosion of biomedical implants, and, at the same time, guarantee a low nickel content on the surface.

Lack of conclusive studies on corrosion behaviour of NiTi under stress and after deformation is academically accepted. It is not yet clear how the NiTi corrosion resistance is affect by different deformation modes. Controversial results point out to an improvement in the corrosion resistance of the alloy after plastic deformation in compression mode whereas plastic deformation achieved by cold-work originates pitting corrosion. Thus, one of the aims of this project is to evaluate the influence of deformation on the corrosion resistance of NiTi. For that propose, corrosion tests will be performed after deformation of the alloy in elastic (up to 8%) and plastic (10 to 25%) domains for various deformation gradients. The assessment of the mechanism that correlates the corrosion behaviour and the mechanical deformation of the alloy is also envisaged.

It is known that a phenomenon of wear-corrosion synergism occurs in body implants due to the simultaneous presence of stress and an aggressive medium. So, the correct evaluation of the corrosion-wear performance of the NiTi and NiTi surface modified alloys is of crucial importance, in order to set the basis for a future selection of the surface modification treatment that induces a better wear-corrosion improvement in service. To simulate wear in an aggressive medium at body temperature, a wear corrosion apparatus is being used at UMinho (pin on plate wear machine coupled with a corrosion cell) to perform a simple configuration reciprocating corrosion-wear test in

human body simulating fluids (Ringer, Hank's or MEM solutions).
The present work deals with the preliminary results of this wide project and, in particular, with those obtained so far from the tribological studies carried out in collaboration with the Centre for Mechanical and Materials Technologies (CT2M) of Universidade do Minho.

INSTALAÇÕES TÉCNICAS EM EDIFÍCIOS – REDES DE AVAC

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Edição: DEM-ISEL/Universidade dos Açores
ISBN: -
Data de Publicação: Abril 2008; pg. 1-57

Com o presente livro pretendo fornecer os conhecimentos pressupostos ao dimensionamento e traçados de redes de fluidos, usualmente utilizadas na distribuição de potência frigorífica/calorífica, em instalações técnicas de edifícios, de acordo com os seguintes pontos:

1. Abordagem à Psicrometria – Propriedades do Ar Húmido, Utilização da Carta Psicrométrica, Processos de Ar Húmido;

2. Sucinta explicitação dos cálculos que estão subjacentes ao projecto e
dimensionamento de sistemas de AVAC – Cálculo de Cargas Térmicas, Sensíveis e Latentes, Factor de Calor Sensível do Local (Linha Característica), Caudal de insuflação;

3. Abordagem ao funcionamento de um ciclo frigorífico e explicação do funcionamento dos seus principais componentes. Definições de COP, EER e principais parâmetros que os condicionam;

4. Sistema de climatização genérico, principais componentes, e suas funções;

5. Classificação de sistemas de AVAC dando particular ênfase aos sistemas centrais a água e multi-sistemas de expansão directa;

6. Demonstração do cálculo automático de cargas térmicas de um local, de um edifício, e das potências necessárias à central, fornecimento de programa de cálculo HAP4.31 da "carrier";

7. Selecção de Unidades de tratamento de ar e ventiloconvectores, Fornecimento do programa de dimensionamento "ABB Airhandling";

8. Selecção de "Chillers" com e sem bomba de calor, fornecimento de programas de selecção;

9. Sistemas de AVAC centrais a água – Dois e Quatro Tubos;

10. Critérios de dimensionamento de redes de distribuição – Perda de carga do sistema;

11. Selecção de grupos electrobomba, fornecimento de programa "WinCAPS 7.44" da "Grundfos";

12. Dimensionamento de redes de sistemas solares térmicos e sua

interligação com sistemas de apoio convencionais;
13. Determinação das espessuras dos isolamentos, fornecimento do programa "ArmWin 3.2" da "Armstrong";
14. Multisistemas de expansão directa – Dimensionamento de redes de fluido frigorigéneo (refrigerante), fornecimento do programa "e-solution" da "Mitsubishi";
15. Dimensionamento de redes de condutas de ar – método da perda de carga constante;
16. Selecção de equipamento de difusão de ar, fornecimento do programa "XSelection Air Diffuser" e Tabelas electrónicas de selecção rápida;
17. Apresentação de esquemas de princípio tipo.

INTELLIGENT TRANSPORT SYSTEM BASED ON RFID AND MULTI-AGENT APPROACHES

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This paper aims at evidence and proposes the use of Radio Frequency Identification (RFID) technologies integrated to an Information and Communication Technologies (ICT) framework. The proposed framework is based on Distributed Artificial Intelligence (DAI) supported by a Multi-Agent System (MAS) approach, as the most value advantage of SCM in cooperative intelligent logistics systems. Furthermore, is proposed that logistical platforms (production or distribution), as nodes of added value of supplying and distribution networks, are the critical points of the visibility of the inventory, where these technological needs are more evident. The book chapter is organized as follows. Section 2 presents the Logistics as an integrated system that includes transportation operations in a worldwide market and presents the concept of SCM giving evidence that enabling technologies support the flows, specially, information flows. In Section 3 authors argue that ICT is a significant source of competitive advantage in SCM, proposing a multi-agent system approach including RFID to cope with the nowadays challenges of global value chains. Section 4 presents a case study and Section 5 provides some concluding remarks.

VEÍCULO AUTÓNOMO PARA TRANSPORTE EM SEGURANÇA DE REFEIÇÕES HOSPITALARES

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O presente invento é um veículo automático para transporte de refeições de locomoção omnidireccional, equipado com sistemas de controlo de temperatura e de gestão de refeições hospitalares, ou de cantinas e outras unidades de restauração.
Este veículo tem incluído um eficiente sistema de informação de dietas personalizadas e permite, por um lado, um transporte seguro das refeições com o controlo de qualidade da contaminação bacteriológica das mesmas, não permitindo a distribuição de refeições se a temperatura sair fora dos níveis de segurança estipulados.
Por outro lado ele garante uma manobrabilidade omnidireccional e a ausência de esforço físico do manobrador, é um veículo que se pode deslocar em todas as direcções com uma total liberdade de movimentos e através de uma condução manual servo-assistida, onde uma pega com sensores detecta a intenção de movimento do operador, sendo o seu deslocamento proporcionado por motores colocados nas rodas. Alternativamente, existe uma versão autónoma, idêntica à apresentada, mas onde o veículo se orienta no espaço e detecta os obstáculos e pessoas através de sensores incorporados no veículo.

FLEXÃO DE ELEMENTOS CURVOS EM MATERIAIS COMPÓSITOS

Leite, Afonso Manuel da Costa de Sousa

Mestrado em: Engenharia Mecânica
Grau Concedido por: Universidade Técnica de Lisboa, Instituto Superior Técnico
Orientador: João Manuel Candeias Travassos
Co-Orientador: Manuel José Moreira de Freitas
Provas Concluídas em: 28 de Maio de 2008

No presente trabalho aborda-se o comportamento mecânico de elementos curvos, em materiais compósitos, aquando sujeitos a forças e momentos nas extremidades. Os seus principais modos de falha são estudados em detalhe: (1) rotura no plano das fibras (falha da matriz ou das fibras) devido às tensões circunferenciais e (2) rotura fora do plano das fibras, por delaminagem, devido às tensões radiais. Foram feitos modelos analíticos e numéricos, validados por experimentação. A solução analítica tem por base a "Teoria Multicamada". Os modelos de Elementos Finitos 3D e 2D foram construídos nos programas LUSAS Composite e ANSYS. Trinta e dois elementos curvos foram fabricados recorrendo ao processo de saco de vácuo em autoclave, usando pré-impregnados unidireccionais de fibra de vidro/resina epoxídica. O seu molde foi também fabricado e maquinado. Quatro elementos curvos foram instrumentados com dois extensómetros cada nas suas faces interna e externa respectivamente. Ensaiaram-se todos os elementos até à ocorrência da primeira falha. Os resultados experimentais foram comparados com os resultados analíticos e numéricos. Para a previsão de rotura aplicaram-se os critérios de Hill 3D e Tsai-Hill em conjunção com o da Tensão Radial Máxima, usando-se as tensões obtidas numericamente.

MULTI-AGENT APPROACH TO FAULT TOLERANT CONTROL SYSTEMS

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Provas Concluídas em: 19 de Dezembro de 2008

A general concern in industrial world is related to process maintenance, safety and functionality problems in the presence of faults. Most industrial processes are very large and/or complex. Because of size and complexity, it is very difficult to conceive a diagnostic system and ensure the availability of the entire process. Sometimes, malfunctions or simple performance deterioration of equipments or processes occur, forcing to production interruptions. Thus, it is fundamental in the industrial world of the 21st century to have Fault Tolerant Control systems, including a Fault Diagnosis system that provides faults information to some kind of control reconfiguration system that will try to accommodate the faults, maintaining the process operation with a minimal degradation in the production or allowing a controlled plant shut down.

As all the industrial processes are physically distributed, heterogeneous and complex, with communication networks forcing a distributed and local vision of the problems, and the need to adapt quickly to changes in the environment structure, it is a proposal of this work the use of Distributed Artificial Intelligence techniques to construct fault tolerant control systems. Thus, this thesis proposes a new architecture for this kind of systems, which takes into account the dimension and complexity of the processes, namely, an architecture based on multi-agent systems. To help in the construction of these systems for industrial processes, a new platform and a new design toolkit for Matlab/Simulink® environment are also proposed. The proposed fault tolerant control system is validated and tested in simulation and in a real three tank process.

UTILIZAÇÃO DE BIOMASSA COMO COMBUSTÍVEL SECUNDÁRIO EM PROCESSOS DE CO-COMBUSTÃO E REBURNING

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Provas Concluídas em: 25 de Março de 2008

Esta tese descreve um estudo experimental sobre a utilização de biomassa como combustível secundário em processos de co-combustão e *reburning* numa fornalha semi-industrial. No caso da co-combustão de combustíveis sólidos com gás natural, começou-se por realizar um extenso conjunto de estudos paramétricos para avaliar o impacto do tipo de combustível sólido e respectiva percentagem na eficiência global da combustão e nas emissões de poluentes. Subsequentemente, foram efectuadas medidas detalhadas das concentrações médias das principais espécies químicas gasosas e temperaturas médias para três chamas representativas. Verificou-se que as emissões de CO, hidrocarbonetos e NO_x aumentam com o aumento da percentagem de combustível sólido, mas que a co-combustão utilizando biomassa pulverizada, mesmo com diâmetros relativamente grandes, permite obter taxas de oxidação do resíduo carbonoso significativamente superiores às obtidas na co-combustão com carvão pulverizado, devido ao elevado teor em matéria volátil presente na biomassa. No caso do *reburning* usando biomassa como combustível secundário, foram inicialmente obtidas medidas detalhadas das concentrações médias das espécies químicas gasosas e temperaturas médias para três chamas distintas, sem *reburning*, com o objectivo de definir a zona adequada de injecção dos combustíveis secundários nos ensaios de *reburning* subsequentes. Posteriormente, foram efectuados estudos paramétricos e medidas detalhadas das concentrações médias das espécies químicas gasosas e temperaturas médias na zona de *reburning* para avaliar a influência de vários parâmetros importantes em processos de *reburning* nas emissões de NO_x e na eficiência global da combustão. Verificou-se que a eficácia do processo de *reburning* usando combustíveis gasosos é geralmente superior à sua eficácia usando combustíveis sólidos, sendo que as emissões de NO_x são significativamente afectadas por parâmetros tais como a fracção de combustível secundário, tempo de residência na zona secundária e granulometria do combustível secundário, independentemente do combustível secundário.

04

ENGENHARIA QUÍMICA

Anuário Científico 2008

ISEL

CATALYTIC CHARACTERIZATION OF PILLARED CLAYS THROUGH TOLUENE METHYLATION REACTION

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Pillared clays (PILCs) with Al and Zr oxide pillars were studied in terms of their structure and texture. The catalytic properties of the samples were evaluated through toluene methylation reaction. As comparison material a commercial zeolite HZSM-5 was used. The toluene conversion at short time-on-stream over PILCs, although smaller than the value obtained with HZSM-5, attains values of 37 (molar %). In all cases the reaction products are a mixture of xylenes, ethyltoluenes and trimethylbenzenes isomers. All samples present higher selectivity to xylene isomers, which are the primary products. For Zr pillared clay the percentage of these isomers is the highest.

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DESENVOLVIMENTO DE NOVOS CATALISADORES PARA A PRODUÇÃO DE BIODIESEL

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Neste trabalho descrevem-se os trabalhos preliminares efectuados sobre o desenvolvimento de novos catalisadores metálicos heterogéneos a serem utilizados na reacção de transesterificação de triglicéridos, que é o processo de obtenção de biodiesel. Actualmente, o biodiesel é correntemente produzido por esta reacção com metanol que é catalisada de forma homogénea, por exemplo, com NaOH ou KOH. Este tipo de catalisadores é corrosivo para os equipamentos, e têm que ser neutralizados após a reacção originando-se, assim, correntes salinas líquidas. Além disso originam uma série de operações de separação que poderão ser obviadas pela utilização de catalisadores heterogéneos e que não originam, também, correntes nem resíduos poluentes.

DEVELOPMENT OF HETEROGENEOUS CATALYSTS FOR TRANSESTERIFICATION OF TRIGHLYCERIDES

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This paper describes preliminary work done towards the development of new metallic heterogeneous catalysts to be used in the transesterification reaction of triglycerides, which is of considerable interest in the production of biodiesel. Biodiesel, is a mixture of mono-alkyl esters of fatty acids, and is currently manufactured by transesterification of triglycerides with methanol using NaOH or KOH as liquid base catalyst. Catalysts as such are corrosive to the equipment, and as these catalysts are present in the liquid phase, must be neutralized after the completion of the reaction, typically using HCl, thus producing salt streams. Moreover, due to the presence of free fatty acids, it reacts to form soaps as unwanted by-products, hence requiring more expensive separation processes. Therefore, there is a great need on the development of industrial processes for biodiesel production using solid acid catalysts. The key benefit of using solid acid catalysts is that no polluting by-products are formed and the catalysts do not have to be removed since they do not mix with the biodiesel product.

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Reaction Kinetics and Catalysis Letters, 2008, 95(2), 273-279.

EMISSIONS OF POLYCICLIC AROMATIC HYDROCARBONS AND POLYCICLIC CARBONYL BIPHENILS FROM ELECTRIC ARC FURNACES

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Publicado em:
Revista de Metalurgia Madrid, 2008, 44(3), 280-284.

This paper describes work done in order to determine the emissions of highly toxic organic micropollutants from electric arc furnaces used in the production of carbon steel from scrap. The study will be allowing to derive relationships between the levels of airborne micropollutants and the operational parameters of the production process so that an abatement of pollution could be achieved.
By using the European standard method CEN 1948 for dioxin like compounds sampling and measurement, it was possible to determine the characteristic fingerprint of micropollutants such as polycyclic aromatic hydrocarbons (PAHs) and PCBs emitted by this particular stationary source.

ESTIMATING LOCAL GREENHOUSE GAS EMISSIONS – A CASE STUDY ON A PORTUGUESE MUNICIPALITY

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This paper describes the study that led to the development of a carbon dioxide emissions matrix for the Oeiras municipality, one of the largest Portuguese municipalities, located in the metropolitan area of Lisbon. This matrix takes into account the Greenhouse Gases (GHG) Emissions, due an increase of electricity demand in buildings as well as solid and liquid wastes treatment, from the domestic and services sectors.

Using emission factors that were calculated from the relationship between the electricity produced and amount of treated wastes, the GHG emissions in the Oeiras municipality, were estimated for a time series of 6 years (1998 to 2003).

The obtained results showed that the electricity sector accounts for about 75% of the municipal emissions in 2003. This study was developed in order to obtain tools to base options and actions to be undertaken by local authorities such as energy planning and also public information.

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International Journal Greenhouse Gas Control, 2008, 2, 130-135.

04

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

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Publicado em:
Ingenium, 2008, 6, 74-79.

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

A GESTÃO INTEGRADA DE RESÍDUOS SÓLIDOS URBANOS – PERSPECTIVA AMBIENTAL E ECONÓMICO--ENERGÉTICA

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A importância dos sistemas integrados de gestão de resíduos sólidos urbanos (RSU) é definida pelos vários componentes processuais desses mesmos sistemas, que são constituídos, basicamente, por tecnologias de operação física, química e biológica. Este artigo, caracteriza estas tecnologias e, o que é extremamente importante, identifica os impactes ambientais mais importantes, associados a estas operações fabris de engenharia. É extremamente importante também, realizar um estudo da viabilidade económica resultante da implementação destas tecnologias e do funcionamento destes sistemas integrados de gestão de RSU, caracterizando quantitativamente as contribuições energéticas de cada uma destas operações. Este estudo foi analisado e os seus resultados são apresentados neste artigo.

Publicado em:
Química Nova, 2008, 31(3), 645-654.

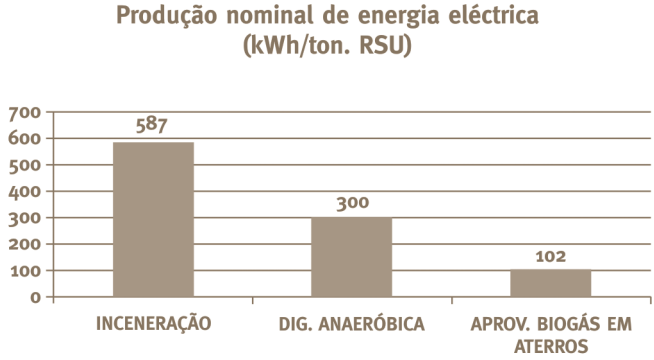

Figura 2. Produção nominal de energia eléctrica para cada método devalorização energética de RSU.

04

A GESTÃO INTEGRADA DE RESÍDUOS SÓLIDOS URBANOS – PERSPECTIVA AMBIENTAL E ECONÓMICO--ENERGÉTICA

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Publicado em:
Química Nova, 2008, 31(3), 645-654.

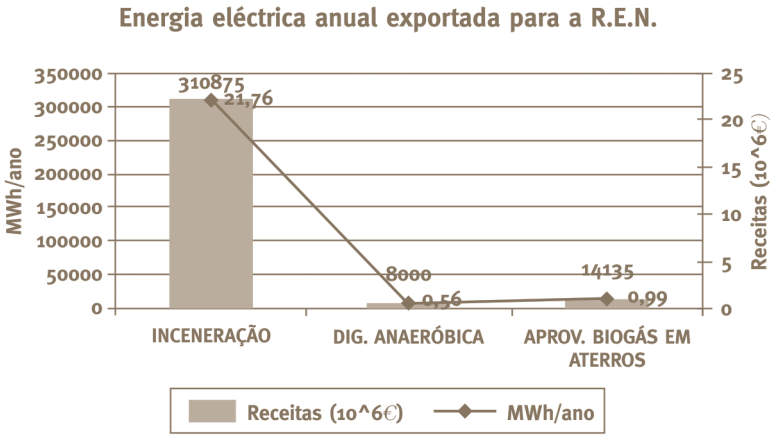

Figura 3. Energia eléctrica anual exportada para a REN e receitas anuais obtidas com a venda dessa energia.

04

HEIGHT OF STACKS WITH LOW POLLUTANT EMISSIONS: ANALYSIS OF DATA FROM A SIGNIFICANT NUMBER OF SMALL AND MEDIUM SIZED INDUSTRIES

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Based on data gathered from a significant number of small and medium sized Portuguese industries, a comprehensive study on the need to heighten stacks with low pollutant emissions is presented. This study considers the application of the recent Portuguese legislation for stack height verification and the application of dispersion modelling tools. The main reasons for stack heightening in existing small and medium sized industries with low pollutant emissions are presented and discussed. The benefits and the environmental impact of the recent Portuguese legislation for stack height verification are discussed.

Publicado em:
Eurasap Newsletter, 2008, 65, 11-20.

n-HEXANE HYDROISOMERIZATION OVER BIFUNCTIONAL Pt/MCM-22 CATALYSTS. INFLUENCE OF THE MODE OF Pt INTRIDUCTION

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Three different methods were used to introduce 1.0 wt.% of Pt in bifunctional Pt/MCM-22 zeolite catalysts: ion exchange with $Pt(NH_3)4^{2+}$, incipient wetness impregnation with $PtCl_6H_2$ and mechanical mixture with Pt/Al^2O^3. The Pt dispersion was estimated by transmission electron microscopy and the hydrogenating activity with toluene hydrogenation at 110°C. From these experiments, it can be concluded that with the ion exchanged sample, platinum was located within the inner micropores and on the outer surface, whereas with the impregnated one, platinum was essentially on the outer surface under the form of large particles. With all the samples there is a fast initial decrease in the activity for n-hexane hydroisomerisation at 250°C. With exchanged and impregnated samples, this decrease is followed by a plateau, the activity value being then higher with impregnated sample. For the sample prepared by mechanical mixture a continuous decrease in activity can be observed. All these differences can be related with the distinct locations of Pt.

AN INVESTIGATION OF THE SYNTHESIS PARAMETERS OF THE REACTION OF HYDROXYAPATITE PRECIPITATION IN AQUEOUS MEDIA

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Hydroxyapatite (HAP), is described 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: $10\ Ca(OH)_2 + 6\ H_3(PO_4) \Leftrightarrow Ca_{10}(PO_4)_6(OH)_2 + 18\ H_2O$. 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.

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04

AN INVESTIGATION OF THE SYNTHESIS PARAMETERS OF THE REACTION OF HYDROXYAPATITE PRECIPITATION IN AQUEOUS MEDIA

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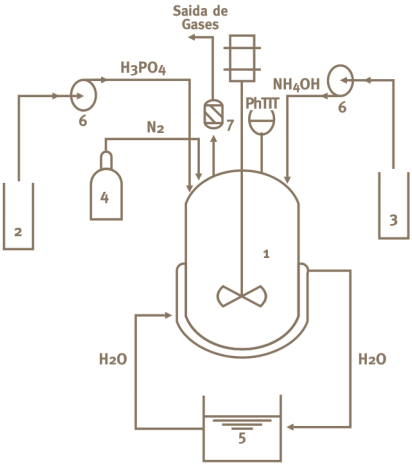
Publicado em:
International Journal Chemical Reactor Engineering, 2008, 6, A103, 1-17.



1. Stirred reactor;
2. Container with orthophosphoric acid (H_3PO_4), 0,3M;
3. Container with ammonia (NH_4OH) a 25%;
4. Nitrogen cylinder (N_2);
5. Heated water bath;
6. Pumps;
7. KOH Filter.

Figure 1. Experimental synthesis apparatus

04

MULTI-OBJECTIVE DESIGN OF REACTIVE DISTILLATION WITH FEASIBLE REGIONS

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This work addresses the multi-objective design of complex reactive distillation columns through the use of feasible regions. A cost indicator reflecting energy usage and column size is introduced and used to build the Pareto surface describing the optimal combinations of cost and performance. The study includes the use of superheated and subcooled feed streams and searches for the optimal distribution of feeds and catalyst inside the column. The technique is first illustrated for a base case system with ideal VLE and then for two variants with different volatilities for reactants and products. The best tradeoff solutions for each system are identified, the operating conditions analyzed and a selected number of cases are investigated further using rigorous simulation in Aspen Plus. Important insights gained and a few heuristic rules about the distribution of the reaction and feed in the column are presented. Furthermore, a methodology that may potentially contribute to overcome limitations on catalyst volume by increasing the specific reaction turnover is presented.

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Industrial & Engineering Chemistry Research, 2008, 47, 7284-7293.

04

A SENSITIVITY ANALYSIS ON OPTIMAL SOLUTIONS OBTAINED FOR A REACTIVE DISTILLATION COLUMN

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Publicado em:
Computer Aided Chemical Engineering, 2008, 25, 211-216.

In previous work (Filipe *et al.* 2007) the multi-objective optimization of a distillation column was performed and the Pareto front relating the total number of stages, reactive holdup and cost, identified. In this work a study on how the Pareto optimal designs could be adapted for real implementation is presented. Different design details, such as reactive holdup and feed quality, are investigated and the sensitivity of the solutions assessed to quantify the effect on the column expected performance.

PERFORMANCE OF SUPPORTED CATALYSTS BASED ON A NEW COPPER VANADATE-TYPE PRECURSOR FOR CATALYTIC OXIDATION OF TOLUENE

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A new copper vanadate precursor with the formula NH4[Cu2.5V2O7 (OH)(2)]center dot H_2O was synthesized and deposited on two different supports, ZSM-5 and amorphous SiO_2, by a hydrothermal method or by mechanical mixture. The catalytic behaviour was evaluated in the total oxidation of toluene and the characterization was performed by H-2-temperature-programmed reduction (H-2-TPR), thermogravimetric analysis, elemental analysis, UV-vis diffuse reflectance spectroscopy and X-ray diffraction.

It was found that the copper vanadate phase comprises two mixed oxides, one of them crystalline, the Ziesite phase, and the other one amorphous. The supported catalysts presented a content of copper vanadate phase of about 9-11 wt.%.

The copper vanadate deposited on ZSM-5 by the hydrothermal method evidences the best performance in the oxidation of toluene. This behaviour can be associated with the smaller size and higher dispersion of the particles on the support, which was confirmed by their better reducibility and higher band gap energy value compared with the other series of studied catalysts.

Publicado em:
Journal of Hazardous Materials, 2008, 153 (1-2), 628-634.

ZEOLITE-COATED CERAMIC FOAMS FOR VOCS REMOVAL

Silva, E.R.[1]; Catalão, R.[1]; Silva, J.M.[1,2]; Vaz, F.[3]; Oliveira, F.[4]; Ribeiro, F.R.[1]; Magnoux, P.[5]; Belin, T.[5]; Ribeiro, M.F.[1]

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Publicado em:
Studies in Surface Science and Catalysis, 2008, 174 (2), 1195-1198.

Copper (Cu) and Platinum (Pt) based MFI catalysts have been supported on cordierite foams by an improved washcoating method. Uniform catalyst coatings with a mean thickness as low as 27 µm presenting a good adherence onto the foam surface (weight losses of about 0.4±0.05 wt.%) were obtained. With catalyst contents around 8–10 wt.%, these coated-foam catalysts revealed better catalytic behaviours than their bulk-form counterparts for the deep oxidation of isopropanol. Conversions into CO_2 of about 100% are reached for the platinum-coated foam at 160°C.

CATALYTIC OXIDATION OF VOLATILE ORGANIC COMPOUNDS WITH A NEW PRECURSOR TYPE COPPER VANADATE

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Catalytic oxidation of toluene in low concentration (800 ppm) in air was carried out over catalysts prepared from a new copper vanadate phase calcined at different temperatures. The catalysts were composed of different crystalline phases, namely ziesite, fingerite, blossite and other copper vanadium oxides. The best catalytic performance was obtained with the material calcined at 320°C (composed of ziesite phase and an amorphous copper vanadium oxide) that showed a light off temperature of 265°C. H_2-TPR measurements indicated that the most active catalysts (calcined at 320 and 400°C) are also the most easily reducible.

Publicado em:
Catalysis Today, 2008, 133-135, 502-508.

04

STRENGTH IMPROVEMENT OF CORDIERITE FOAMS BY A DIP COATING METHOD

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Publicado em:
Advanced Materials Forum IV, Materials Science Forum, 2008, 587-588, 123-127.

The structure and morphological aspects of highly porous (higher than 90%) cordierite (Mg2Al4Si5O18) foams, prepared by a direct foaming method, have been evaluated by Scanning Electron Microscopy analysis. The resulting ceramic foams consisted of a three-dimensional array of struts forming a well-defined open-cell structure. This type of structure seems very attractive for catalyst support purposes. Attempts have been made in order to control the pore structure since it directly affects the physical properties, namely the mechanical strength. In this respect, the use of a dip coating method to improve the strength of the resulting foams was found to be effective in reducing defects (e.g. pores, flaws) in the struts. Based on image analysis, estimated mean cell sizes were about 550 mu m whereas strut thicknesses varied in the range of 60-70 mu m. The compressive strength of the developed foams increased by one order of magnitude (0.1 to 1 MPa) by increasing the relative density from 0.06 to 0.18.

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

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

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International Journal of Environmental Studies, 2008, 65(6), 755-767.

SOLAR ACTIVITY AS A POSSIBLE CAUSE OF LARGE FOREST FIRES – A CASE STUDY: ANALYSIS OF THE PORTUGUESE FOREST FIRES

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Fires of large dimension destroy forests, harvests and housing objects. Apart from that combustion products and burned surfaces become large ecological problems. Very often fires emerge simultaneously on different locations of a region so a question could be asked if they always have been a consequence of negligence, pyromania, high temperatures or maybe there has been some other cause. This paper is an attempt of establishing the possible connection between forest fires that numerous satellites registered and activities happening on the Sun immediately before fires ignite. Fires emerged on relatively large areas from Portugal and Spain on August 2005, as well as on other regions of Europe. The cases that have been analyzed show that, in every concrete situation, an emission of strong electromagnetic and thermal corpuscular energy from highly energetic regions that were in geo effective position had preceded the fires. Such emissions have, usually, very high energy and high speeds of particles and come from coronary holes that also have been either in the very structure or in the immediate closeness of the geo effective position. It should also be noted that the solar wind directed towards the Earth becomes weaker with deeper penetration towards the topographic surface. However, the results presented in this paper suggest that, there is a strong causality relationship between solar activity and the ignition of these forest fires taking place in South-western Europe.

SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF VOLATILE OIL FROM ITALIAN CORIANDER SEEDS

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Supercritical CO_2 fluid extraction of the volatile oil from Italian coriander seeds was carried out under different conditions of temperature (40 and 50°C), pressure (90, 100 and 150 bar), mean particle size (0.4, 0.6 and 0.8 mm) and CO_2 flow rate (0.79, 1.10 and 1.56 kg/h) in order to evaluate their influence on the yield and composition of the volatile oil. Hydrodistillation with the same mean particle sizes was performed and used as a comparative method. The best supercritical fluid extraction conditions were found to be 90 bar, 40°C, 1.10 kg/h and 0.6 mm. The chemical composition of each supercritical fluid extraction sample was analysed by GC and GC–MS and the global composition was compared with that obtained by hydrodistillation. The dominant components were linalool (65–79%), c-terpinene (4–7%), camphor (3%), geranyl acetate (2–4%), a-pinene (1–3%), geraniol (1–3%) and limonene (1–2%). Moreover, supercritical fluid extraction samples were collected at specific intervals of amount of CO_2 consumed, during each extraction, and the contribution of the main volatile components from each sample, for the global volatile compositions, was evaluated. In general, the first sample of each extraction contained up to 50% of the mass of each component.

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Food Chemistry, 2008, 111(1), 197-203.

04

VISCOSITY MEASUREMENTS OF COMPRESSED LIQUID REFRIGERANT BLEND R-507A, USING A VIBRATING-WIRE TECHNIQUE

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J. Chem. Eng. Data, 2008, 53, 53-56.

The refrigerant blend R-507A (50 wt % HFC-143a, 50 wt % HFC-125) is an azeotropic mixture of hydrofluorocarbon refrigerants, 1,1,1 trifluoroethane (HFC-143a) and pentafluoroethane (HFC-125). The paper reports viscosity measurements, performed with a vibrating-wire viscometer, of the refrigerant blend R-507A, at five temperatures in the range (253 to 293) K. The measurements were carried out at pressures from slightly above saturation up to 10 MPa, except for the isotherms at 253.26 K where the maximum pressure was 7.52 MPa and at 263.23 K where the maximum pressure was 7.09 MPa. The overall uncertainty of these measurements is estimated to be (1.0%. The data obtained were correlated by means of a modified hard-sphere based correlation technique. The root-mean-square deviation, rmsd, of the experimental results from the correlation equations is 0.23%, and their bias is not significant. This correlation method has also been used to interpolate and extrapolate the present results to enable comparisons with measurements performed by other authors of the viscosity of liquid R-507A at different temperatures and pressures.

SYNTHESIS OF ORGANOMETALLIC Ru(II) AND Fe(II) COMPLEXES CON-TAINING FUSED RINGS HEMI-HELICAL LIGANDS AS CHROMOPHORES. EVALUATION OF NONLINEAR OPTICAL PROPERTIES BY HRS

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A new family of three-legged piano stool structured organometallic compounds containing the fragment η^5-cyclopentadienylruthe-nium(II) /iron(II) has been synthesized to evaluate the existence of electronic metal to ligand charge transfer upon coordination of the novel benzodithiophene ligands (BDT), benzo[1,2-*b*;4,3-*b*']dithiophen-2-carbonitrile (**L1**) and benzo[1,2-*b*;4,3-*b*']dithiophen-2'nitro-2-carbo-nitrile (**L2**). All the compounds were characterized by ^{1}H, ^{13}C, ^{31}P NMR, IR and UV–Vis. Spectroscopies and their electrochemistry studied by cyclic voltammetry. The X-ray structures of $[Ru(\eta^5\text{-}C_5H_5)(PPh_3)_2\text{-}(NCC_{10}H_5S_2)][PF_6]$ (**1Ru**), $[Ru(\eta^5\text{-}C_5H_5)(PPh_3)_2(NCC_{10}H_5S_2)][CF_3SO_3]$ (**1'Ru**), $[Ru(\eta^5\text{-}C_5H_5)(DPPE)(NCC_{10}H_5S_2)][PF_6]$ **2Ru** and $[Fe(\eta^5\text{-}C_5H_5)(DPPE)(NCC_{10}H_5S_2)][PF_6]$ (**2Fe**) were determined by X-ray diffraction showing centric crystallization on groups P_1 and $P2_1/n$, respectively.
Quadratic hyperpolarizabilities (β) of some of the complexes (**2Fe**, **2Ru** and **3Fe**) have been determined by hyper-Rayleigh scattering (HRS) measurements at a fundamental wavelength of 1500 nm, to minimize the probability of fluorescence due to two-photon absorption and to reduce the effect of resonance enhancement, in order to estimate static β values.

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Journal of Organometallic Chemistry, 2008, 693, 2987-2999.

04

STUDIES TOWARD THE LIVING POLYMERIZATION OF PHENYLETHYNYL-CALIX[4]ARENE COMPOUNDS WITH RH-BASED TERNARY CATALYTIC SYSTEMS

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Publicado em:
Supramolecular Chemistry, 2008, 20, 95-108.

The living polymerization of mono and difunctional-phenylethynylcalix[4]arene compounds **1** and **2** by Rh(I) ternary catalytic systems (TCS) was examined. Two TCS were tentatively prepared *in situ*, adapting known methodologies: (a) Rh(C CPh) (norbornadiene) (PPh_3) and (b) Rh(C(Ph)C=CPh_2)(norbornadiene)(PPh_3). Using the first TCS, the conjugated polymers **poly 1** and **poly 2** could be obtained in very good yields (77-86%), in short reaction times and freed from low molecular-weight products, only when NEt_3 was used as a co-catalyst. With the second TCS, excellent results were obtained. Indeed, this catalytic system proved quite efficient in the polymerization of calix[4]arenes **1** and **2**, affording the correspondent **poly 1** and **poly 2** essentially in almost quantitative yields (by GPC analysis), under appropriate conditions. The living nature of the polymerization has been proved. For instance, in the case of calix[4]arene **1**, the M_n of the polymer obtained at high monomer conversion, increased proportionally with the [**1**]:[Rh] molar ratio in the feed, keeping $[\mathbf{1}]_0$ constant, thus showing that irreversible chain transfer or termination reactions did not occur to a major extent. Under the most favorable conditions {[**1**]:[Rh]=50 and [**2**]:[Rh]=50}, the polydispersities of **poly 1** and **poly 2** were kept in a narrow range (1.16-1.30).

NOVEL FLUORESCENT (P-PHENYLENE ETHYNYLENE)-CALIX[4]ARENE-BASED POLYMER DESIGN, SYNTHESIS AND PROPERTIES

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Publicado em:
J. Polym. Sci. Pol. Chem. A, 2008, 46, 6477-6488.

A novel fluorescent (*p*-phenylene ethynylene)-calix[4]arene-based polymer (**CALIX-PPE**) has been successfully synthesized by cross-coupling polymerization of bis-calix[4]arene **1** with 1,4-diethynylbenzene. The polycondensation was carried out in toluene/NEt_3 at 35°C for 24h, using $PdCl_2(PPh_3)_2$/CuI as the catalytic system, furnishing **CALIX-PPE** in excellent isolated yields (higher than 95%, several runs). The yellow polymer is freely soluble in several nonprotic organic solvents. The GPC trace of the isolated polymer showed a monomodal distribution and a number average molecular weight of 23300 gmol-1 (M_w/M_n= 2.05). No evidence was found in the structural analysis (FTIR and $^1H/^{13}C$ NMR) regarding the formation of alkyne homocoupled segments along the polymer chain. For comparative purposes, the synthesis of an analogous poly(*p*-phenylene ethynylene) containing *p-t*-butyl-phenoxymethyl side chains (**TBP-PPE**) was also undertaken. A great similarity was found between the photophysical properties of **CALIX-PPE** and **TBP-PPE** in solution (UV-Vis and laser induced luminescence), clearly demonstrating their unique dependence on the structure and conformation of the conjugated PPE backbone. The fluorescence spectra of polymers are of nearly identical shape, displaying their maximum emission around 420 nm. The calculated solution photoluminescence quantum yields of **CALIX-PPE** and **TBP-PPE** are of similar magnitude (ϕ_F (**CALIX-PPE**)= 0.43; ϕ_F (**TBP-PPE**)= 0.51).

04

HALF-SANDWICH SCORPIONATE VANADIUM, IRON AND COPPER COMPLEXES: SYNTHESIS AND APPLICATION IN THE CATALYTIC PEROXIDATIVE OXIDATION OF CYCLOHEXANE UNDER MILD CONDITIONS

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Publicado em:
Advanced Synthesis and Catalysis, 2008, 350, 706-716.

The new half-sandwich scorpionate complexes $[VCl_3\{HC(pz)_3\}]$ **1** (pz = pyrazolyl), $[VCl_3\{SO_3C(pz)_3\}]$ **2**, $[FeCl_2\{HC(pz)_3\}]$ **3**, $Li[FeCl_2\{SO_3C(pz)_3\}]$ **4** and $[CuCl\{SO_3C(pz)_3\}]$ **5** were synthesized, characterized and shown to act, as well as the related $[CuCl_2\{HC(pz)_3\}]$ **6**, as selective catalysts (or catalyst precursors) for the peroxidative oxidation (by H_2O_2) of cyclohexane to cyclohexanol and cyclohexanone, under mild conditions (at room temperature and using an aqueous solution of H_2O_2). The iron complexes are the most active ones (reaching TON values up to *ca.* 690), the effects of a variety of factors are reported and the reaction is shown to proceed via both C- and O-centred radical mechanisms, conceivably involving a metal-based oxidant.

CYCLOHEXANE OXIDATION WITH DIOXYGEN CATALYZED BY SUPPORTED PYRAZOLE RHENIUM COMPLEXES

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The pyrazole complexes $[ReCl_2\{N_2C(O)Ph\}(Hpz)(PPh_3)_2]$ **2** (Hpz = pyrazole), $[ReCl_2\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ **3** and $[ReClF\{N_2C(O)Ph\}(Hpz)_2(PPh_3)]$ **4**, and their precursor $[ReOCl_3(PPh_3)_2]$ **1**, immobilized on 3-aminopropyl functionalized silica, catalyze the cyclohexane oxidation with dioxygen, to cyclohexanol and cyclohexanone (the main product), in the absence of solvent and additives and under relatively mild conditions. Complex 4, whose synthesis and characterization are reported herein for the first time, provides the best activity (*ca.* 16 % overall conversion towards the ketone and alcohol, at the O_2 pressure of 19 atm, at 150°C, 8 h reaction time). The reaction is further promoted by pyrazinecarboxylic acid. TGA analysis shows that the supported complexes are stable up to ca. 200°C. The use of radical traps supports the involvement of a free-radical mechanism via carbon- and oxygen-centred radicals. The effects of various factors were studied towards the optimization of the processes. Complex **4** also catalyses the oxidation of other cycloalkanes to the corresponding cycloalkanols and cycloalkanones.

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04

Cu(I) COMPLEXES BEARING THE NEW STERICALLY HINDERED AND COORDINATION FLEXIBLE TRIS (3-PHENYL-1-PYRAZOLYL) METHANESULFONATE ($TPMS^{Ph}$) LIGAND AND THE WATER-SOLUBLE PHOSPHINE 1,3,5-TRIAZA-7-PHOSPHAADAMANTANE (PTA) OR RELATED LIGANDS

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The new sterically hindered scorpionate tris(3-phenylpyrazolyl) methanesulfonate ($Tpms^{Ph}$)$^-$ has been synthesized and its coordination behavior toward a Cu(I) center, in the presence of 1,3,5-triaza-7-phosphaadamantane (PTA), *N*-methyl-1,3,5-triaza-7-phosphaadamantane te-traphenylborate ((Me-PTA)[BPh_4]) or hexamethylenetetramine (HMT) has been studied. The reaction between Li($Tpms^{Ph}$) **1** and [$Cu(MeCN)_4$][PF_6] yields [Cu($Tpms^{Ph}$)(MeCN)] **2** which, upon further acetonitrile displacement on reaction with PTA, HMT or (Me-PTA)[BPh_4], gives the corresponding complexes [Cu($Tpms^{Ph}$)(PTA)] **3**, [Cu($Tpms^{Ph}$)(HMT)] **4** and [Cu($Tpms^{Ph}$) (Me-PTA)][PF_6] **5**. All the compounds have been characterized by ^1H, ^{31}P, ^{13}C, COSY or HMQC-NMR, IR, elemental analysis and single crystal X-ray diffraction. In the complexes **3** and **5**, which bear a phosphine ligand (*i.e.* PTA and Me-PTA, respectively), the new scorpionate ligand shows the typical N,N,N-coordination mode, where as in **2** and **4**, bearing a N-donor ligand (*i.e.* MeCN and HTM, respectively), it binds the metal via the N,N,O chelating mode, involving the sulfonate moiety.

PRODUCTION OF LACCASE AND XYLANASE FROM Coriolus versicolor GROWN ON TOMATO POMACE AND THEIR CHROMATOGRAPHIC BEHAVIOUR ON IMMOBILIZED METAL CHELATES

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A strain of *Coriolus versicolor* was grown in tomato pomace as sole carbon source for the production of laccase and xylanase. This culture exhibited a peak of laccase (362 U/L of fermentation broth) and xylanase (2565 U/L of fermentation broth) activities on the 3rd and 14th day of cultures with a specific activity of 3.7 and 11.7 U/mg protein, respectively. Differential chromatographic behaviour of xylanase and laccase from C. versicolor was investigated on immobilized metal chelates. The effect of pH, length of spacer arm, the presence of imidazole and nature of metal ion was studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). PDB survey of solvent accessible histidine residues in laccase and xylanase families was carried out by using bioinformatic tools. A one-step purification for laccase from *C. versicolor* was devised by using Sepharose 6B–EPI 30–IDA–Cu(II) and the purified enzyme was obtained with a specific activity of about 15.0 U/mg protein, a final recovery of enzyme activity of about 60% and a purification factor of about 10. The purified preparation of laccases A exhibited an optimum pH of activity of 5.0 and 3.0 with odianisidine and ABTS as substrates, respectively. The optimum temperature of activity for this enzyme was found to be 80 8C in acetate buffer at pH 4.5 whereas the half-life (t1/2) of 19.4 ± 2.2 h and 0.50 ± 0.012 h was obtained at 45 and 60 8C, respectively. The kinetic parameters (V_{max}, K_m, K_{cat} and K_{cat}/K_m) of the purified enzyme were also obtained with o-dianisidine, guaiacol and ABTS as substrates. By using selective experimental conditions in IMAC, it was possible to separate successfully laccase isoenzymes into two groups, one with low and the other with high pI values. Kinetic characterization of both groups of isoenzymes was also carried out.

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04

PRODUCTION AND CHROMATOGRAPHIC BEHAVIOUR OF POLYGALACTURONASE FROM Pleurotus ostreatus ON IMMOBILIZED METAL CHELATES

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A strain of *Pleurotus ostreatus* was grown in submerged culture in tomato pomace as sole carbon source for production of polygalacturonase. The culture of *P. ostreatus* revealed a peak of polygalacturonase activity (2181 U/l) on 4th day with specific activity of 42.8 U/mg protein. Differential chromatographic behaviour of polygalacturonase, xylanase and laccase from P. ostreatus was investigated on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion was studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The presence of imidazole in the equilibration buffer abolished the adsorption of the enzymes to immobilized metal chelates. A one-step purification of polygalacturonase from *P. ostreatus* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II). Purified enzyme exhibited a specific activity of about 1600 U/mg protein, final recovery of enzyme activity of 80% and a purification factor of about 65. The purified enzyme preparation was analysed by SDS-PAGE as well as by in situ detection of enzyme activity. Purified preparation of polygalacturonase exhibited a pH and temperature optima of activity at 7.0 and at 50 8C, respectively. The kinetic parameters (V_{max}, K_m, K_{cat} and K_{cat}/K_m) of purified enzyme were found to be 5530.8 ± 260.7 U/mg of protein, 13.23 ± 2.79 mg/ml of polygalacturonic acid, 5553.01 ± 261.7 s^{-1} and 419.72 s^{-1} mg^{-1}, respectively. Purified enzyme exhibited a half-life (t 1/2) of 60 ± 7.45 min and 35 ± 0.37 min at 50°C and at pH 6.0 and 7.0, respectively.

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

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Publicado em:
J Ind Microbiol Biotechnol, 2008, 35, 475–484.

Tomato pomace and pectin were used as the sole carbon sources for the production of polygalacturonase from a strain of *Coriolus versicolor* in submerged culture. The culture of *C. versicolor* grown on tomato pomace exhibited a peak of polygalacturonase activity (1,427 U/l) on the third day of culture with a specific activity of 14.5 U/mg protein. The production of polygalacturonase by *C. versicolor* grown on pectin as a sole carbon source increased with the time of cultivation, reaching a maximum activity of 3,207 U/l of fermentation broth with a specific activity of 248 U/mg protein. The levels of different isoenzymes of polygalacturonase produced during the culture growth were analysed by native PAGE. Differential chromatographic behaviour of lignocellulosic enzymes produced by *C. versicolor* (*i.e.* polygalacturonase, xylanase and laccase) was studied on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion were studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The adsorption of these lignocellulosic enzymes onto immobilized metal chelates was pH-dependent since an increase in protein adsorption was observed as the pH was increased from 6.0 to 8.0. The adsorption of polygalacturonase as well as other enzymes to immobilized metal chelates was due to coordination of histidine residues which are available at the protein surface since the presence of imidazole in the equilibration buffer abolished the adsorption of the enzyme to immobilized metal chelates. A one-step purification of polygalacturonase from *C. versicolor* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II) and purified enzyme exhibited a specific activity of about 150 U/mg protein, final recovery of enzyme activity of 100% and a purification factor of about 10. The use of short spacer arm and the presence of imidazole in equilibration buffer exhibited a higher selectivity for purification of polygalacturonase on this column with a high purification factor. The purified enzyme preparation was analysed by SDS-PAGE as well as by "*in situ*" detection of enzyme.

ASSESSMENT OF SACCHARIDE FRACTIONATION BY ULTRAFILTRATION AND NANOFILTRATION

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This paper addresses the investigation of the fractionation of saccharide mixtures and saccharide mixtures with calcium using ultrafiltration (UF) and nanofiltration (NF). A set of cellulose acetate membranes covered a wide range of molecular weight cut-off (MWCO) ranging from 250 to 46,000 Da and the total feed concentration of saccharides mixtures varied from 1550 to 4700 ppm with the ratio of the two saccharides-solutes (glucose to raffinose) being kept constant at the value of 1.8. The evolution pattern of the saccharide concentration ratio in the UF/NF permeate streams displayed a dependence on the membrane MWCO, on the total sugar concentration and on the presence of calcium ions. For the highest total sugar content, the membranes with MWCO from 2000 to 7000 Da showed saccharide fractionation capability that was enhanced in the presence of calcium.
The Steric Pore Flow Model was used to predict individual solute permeation behaviours and to assess the deviations to steric hindered transport of the solutes in multi-component saccharide solutions.

A POTENTIOMETRIC BIOSENSOR FOR ACRYLAMIDE AND FORMAMIDE QUANTIFICATION IN WASTEWATER USING WILD-TYPE AMIDASE FROM *Pseudomonas Aeruginosa*

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Acrylamide is an amide with potentially hazardous effects on environment and human health. Humans exposed to acrylamide have revealed symptoms such as muscular weakness, skin and mucous irritation, nausea and numbness. In addition acrylamide is a potent neurotoxin that can cause serious nervous system damage. Long term exposure to this chemical may also be responsible for several types of cancer.

Environmental effects may include death of animals, birds and fish, and death or low growth rate in plants. Accumulation in groundwater may also occur, as well as persistence in aquatic environments [1, 2]

Acrylamide is mainly used in the production of water-soluble polymers used as additives for drinking water, in enhanced oil recovery, in wastepaper recycling, as soil conditioning agents, in sewage and waste treatment, in the synthesis of dyes, in textile industry, as copolymers for contact lenses and in the construction of dam foundations, tunnels, and sewers.

On the other hand acrylamide forms in certain foods, particularly plant-based foods that are rich in carbohydrates and low in protein, during processing or cooking at high temperatures.

Like acrylamide, formamide is an amide that may pose serious environmental and human health effects. In this regard it is essential to develop methods in order to determine, reduce and control the amount of acrylamide and/or formamide present in the environment, namely wastewater [3], as well as in food, human and animal organisms.

Our group has been working in the development of a potentiometric biosensor [5] in order to determine the amount of these amides in environmental and food samples. The biosystem consists in whole cells of *Pseudomonas aeruginosa* containing intracellular amidase activity instead of the traditional use of cellular extract. In the construction of the biosensor, the cells are immobilized [5] on the surface of a polyethersulphone membrane in the presence of glutaraldehyde as bifunctional reagent. This membrane is then attached to the surface of an ammonium ion selective electrode [6].The reaction that

occurs is the hydrolysis of formamide or acrylamide (catalyzed by amidase), with formation of formic or acrylic acid, respectively, and ammonium ion which is potentiometric measured by the ammonium ion selective electrode.
The results obtained revealed excellent analytical characteristics of the biosensor such as linear concentration range for formamide and acrylamide, sensitivity, repeatability, response time and stability, for synthetic as well as for real environmental samples, namely wastewater samples. Furthermore the half-life time of the biosensor obtained for acrylamide was about 18 days. Presently our investigation aims the optimization of the biosensor half-life time for acrylamide as well as for formamide.

BIOCATALYSIS IN ORGANIC MEDIA BY USING CALIXARENE-MYOGLOBIN COMPLEX WITH PSEUDOACTIVITY OF PEROXIDASE

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The present work involves the use of *p-tert*-butylcalix[4,6,8]arene carboxylic acid derivatives for selective extraction of myoglobin. All three calixarenes were found to extract this haemoprotein to organic phase, exhibiting extraction parameters higher than 0.90. Myoglobin-^{t}butyl[6]CH_2COOH complex revealed pseudoactivity of peroxidase which catalysed the oxidation of seryngaldazine in the presence of hydrogen peroxide in organic medium containing chloroform. The effect of pH, protein and substrate concentrations was investigated in biocatalysis by using myoglobin-^{t}Butil[6]CH_2COOH complex. The highest specific activity of myoglobin was 1.37 x 10^{-1} U. mg protein^{-1} at initial pH of 6.5 in organic medium. Apparent kinetic parameters ($V'_{máx}$, K'_m, k'_{cat} e k'_{cat}/K'_m) for the pseudo-activity of peroxidase were determined in organic media for different pH values by Michaelis-Menten. Furthermore, the stability of the protein-calixarene complex was investigated for different initial pH values and $t_{1/2}$ values were obtained in the range of 3.5 – 5.2 days. Myoglobin-calixarene complex present in organic medium was recovered in fresh aqueous solutions at alkaline pH, with a recovery of pseudo-peroxidase activity of over 100%. The results strongly suggest that the use of calixarene derivatives is an alternative technique for protein extraction and solubilisation in organic media for biocatalysis.

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Proceedings da 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Braga, 4 a 6 de Setembro de 2008, pp. 1896-1901.

ONE-STEP PURIFICATION OF HEMOGLOBIN FROM HUMAN ERYTHROCYTES BY USING A NOVEL CHROMATOGRAPHIC MATRIX BASED ON POLYMER-BOUND CALIX[6]ARENES

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Calixarenes are host molecules which exhibit molecular recognition towards a wide range of guest bioactive substances such as amino acids, proteins and carbohydrates. Calix[n]arenes consist of cavity-shaped architecture which can form host-guest complex with a wide range of guest molecules by introducing several functional groups either at the upper or lower rim.

The present work involves the use of a novel chromatographic matrix based on repeating units of *p-tert*-butylcalix[6]arene carboxylic acids for one-step isolation of haemoglobin from human erythrocytes. The red cell lysate was applied to a column packed with this matrix which was previously equilibrated in phosphate buffer. The adsorbed proteins were eluted from the column with a linear gradient of Na_2CO_3 pH 11.0 and the column fractions were analysed for protein and pseudoactivity of peroxidase. Human haemoglobin was purified in a one-step procedure with a recovery of pseudoactivity of about 35% and a purification factor of about 12. The purified haemoglobin was analysed both by SDS and native PAGE which exhibited single proteins bands with Mr of 16.0 and 61.0 kDa, respectively. Furthermore, the single protein band observed in native PAGE was coincident with the pseudo-activity of peroxidase band detected *in situ* on this gel. Protein adsorption on this novel chromatographic matrix involved several interactions such as electrostatic and hydrophobic and other parameters affected this process such as protein size, pI, pH, ionic strength and nature of buffer.

These results strongly suggest that this novel chromatographic matrix presents some advantages over other matrices as far as selectivity is concerned for protein purification.

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

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Tomato pomace and pectin were used as the sole carbon sources for production of polygalacturonase from a strain of *Coriolus versicolor* in submerged culture. The culture of *C. versicolor* grown on tomato pomace exhibited a peak of polygalacturonase activity (1427 U/L) on the 3rd day of culture with a specific activity of 14.5U/mg protein. The production of polygalacturonase by *C. versicolor* grown on pectin as sole carbon source, increased with the time of cultivation, reaching a maximum activity of 3207 U/L of fermentation broth with a specific activity of 248 U/mg protein. Differential chromatographic behaviour of lignocellulosic enzymes produced by *C. versicolor* (*i.e* polygalacturonase, xylanase and laccase) was studied on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion were studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The adsorption of polygalacturonase as well as other enzymes to immobilized metal chelates was due to coordination of histidine residues which are available at the protein surface since the presence of imidazole in the equilibration buffer abolished the adsorption of the enzyme to immobilized metal chelates. A one-step purification of polygalacturonase from *C. versicolor* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II) and purified enzyme exhibited a specific activity of about 150 U/mg protein, final recovery of enzyme activity of 100% and a purification factor of about 10. The use of short spacer arm and the presence of imidazole in equilibration buffer exhibited a higher selectivity for purification of polygalacturonase on this column with a high purification factor. The purified enzyme preparation was analysed by SDS-PAGE as well as by "*in situ*" detection of enzyme activity.

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DEVELOPMENT OF A BIOSENSOR BASED ON ION-SELECTIVE ELECTRODE FOR UREA IN MILK BY USING IMMOBILIZED AMIDASE FROM Pseudomonas aeruginosa

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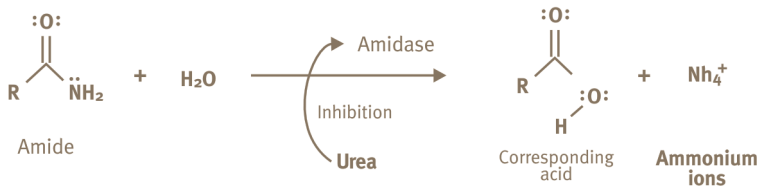
The present work involves the development of a biosensor based on ion-selective electrode (ISE) for assay of urea in milk by using a novel enzymatic method. Urea is a powerful time-dependent active-site directed inhibitor for aliphatic amidase (acylamide amidohydrolase EC 3.5.1.4) from *Pseudomonas aeruginosa* which catalyses the hydrolysis of a small number of aliphatic amides producing the corresponding acid and ammonia (Martins *et. al.* 2006; Tata *et. al.*, 1994) according to the following reaction:



Increasing concentrations of urea were found to inhibit proportionally amidase activity which was detected by the hydrolase reaction. Therefore, urea concentration in samples was inversely proportional to amidase activity which was measured with acetamide as substrate by using ISE for ammonium ions.

Cell-free extracts containing amidase activity were immobilized on nylon and polyethersulfone membranes in the presence of gelatin and glutaraldheyde as the bifunctional reagent. Membranes containing immobilized amidase activity were used to set up a biosensor based on ISE for ammonium ions by using acetamide as the substrate and the enzyme reaction was followed by measurement of ammonium ions due to hydrolysis of the aliphatic amide (Fig.1)

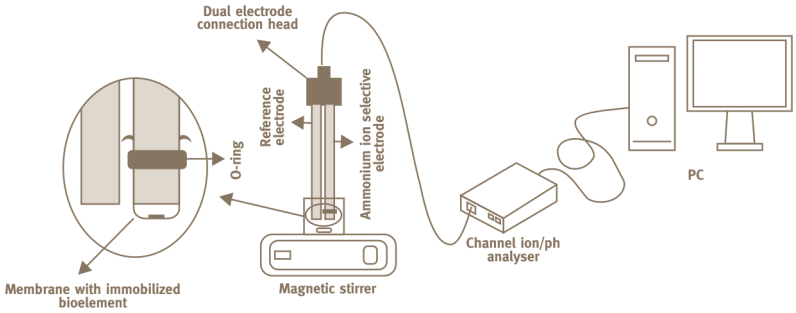


Figure 1. Experimental set-up for potentiometric biosensor: ammonium ion selective electrode containing polyethersulfone membrane with immobilized cell-free extract and reference electrode, electrochemical cell, magnetic stirrer, ISE analyser and PC.

Subsequently, this biosensor was washed and incubated with milk containing increasing concentrations of urea in the range of 0 – 1.0 mM, for 1h. After the incubation period, the biosensor containing amidase activity was assayed again by using acetamide as the substrate. There was a linear relationship between a decrease of the biosensor response in mV and urea concentration in milk. This biosensor exhibited a linear response in the range of 2.0 –10.0 x 10^{-6} M of urea either in a buffer solution or in milk and a response time of 60 s. The biosensor containing amidase activity could be re-used again by reactivating enzyme activity with hydroxylamine for 2h. This biosensor was stable for at least 1month since it did not lose enzyme activity and it is cheap because cell-free extracts containing amidase activity can be used for quantification of urea in milk.

PRODUCTION AND CHROMATOGRAPHIC BEHAVIOUR OF POLYGALACTURONASE FROM Pleurotus ostreatus ON IMMOBILIZED METAL CHELATES

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Proceedings da 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Braga, 4 e 6 de Setembro de 2008, pp. 1913-1918.

A strain of *Pleurotus ostreatus* was grown in submerged culture in tomato pomace as sole carbon source for production of polygalacturonase. The culture of P. ostreatus revealed a peak of polygalacturonase activity (2181 U/L) on 4th day with specific activity of 42.8 U/mg protein. Differential chromatographic behaviour of polygalacturonase, xylanase and laccase from *P. ostreatus* was investigated on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion was studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The presence of imidazole in the equilibration buffer abolished the adsorption of the enzymes to immobilized metal chelates. A one-step purification of polygalacturonase from *P. ostreatus* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II). Purified enzyme exhibited a specific activity of about 1600 U/mg protein, final recovery of enzyme activity of 80% and a purification factor of about 65. The purified enzyme preparation was analysed by SDS-PAGE as well as by *in situ* detection of enzyme activity. Purified preparation of polygalacturonase exhibited a pH and temperature optima of activity at 7.0 and at 50°C, respectively. The kinetic parameters (V_{max}, K_m, K_{cat}, and K_{cat}/K_m) of purified enzyme were found to be 5530.8 ± 260.7 U/mg of protein, 13.23 ± 2.79 mg/ml of polygalacturonic acid, 5553.01 ± 261.7s^{-1} and 419.72 $s^{-1}.mg^{-1}$, respectively. Purified enzyme exhibited a half life (t 1/2) of 60 ± 7.45 min and 35 ± 0.37 min at 50°C and at pH 6.0 and 7.0, respectively.

04

ANALYSIS OF PRODUCTION OF RECOMBINANT WILD-TYPE AMIDASE FROM Pseudomonas aeruginosa IN Escherichia coli

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This work reports on the optimization of a recombinant *Pseudomonas aeruginosa* amidase (E.C.3.5.1.4) production in an *Escherichia coli* strain. The effect of several parameters such as temperature incubation, IPTG induction and ethanol shock on the enzyme aggregation *in vivo* was investigated. The results have demonstrated the formation of inclusion bodies at all the experimental conditions with the highest yield of soluble amidase relatively to other proteins obtained for the condition at 37°C using 0.40 mM IPTG to induce growth with ethanol. Our findings showed that the addition of ethanol in LB ampicillin culture medium at 25°C allowed the production of high levels of amidase but which aggregated quantitatively in a biological active form and exhibited a four-fold higher specific activity when compared with the soluble form of the enzyme. Nondenaturing solubilization of the aggregated amidase was achieved using L-arginine with the highest yield of enzyme solubilization obtained when using a concentration of 2 M. Conversely GdnHCl did not succeed in the denaturing solubilization of amidase inclusion bodies.

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OVERPRODUCTION OF PROTEIN-BOUND POLYSACCHARIDES FROM A *Coriolus versicolor* STRAIN BY SUBMERGED FERMENTATION

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Some mushroom strains are able to synthesize polysaccharopeptides with antitumoral and immunostimulating properties. The aim of this study was to define experimental conditions to optimize the production of protein-bound polysaccharides by *Coriolus versicolor*. In order to evaluate and to optimize the production of these compounds, submerse cultures were performed with four different carbon sources: glucose, maltose, sucrose and mannitol.

Additionally, aiming for a clean process and to reduce the medium cost, two kinds of agroindustrial residues were used: tomato pomace and beet wastes.

The highest polysaccharide concentration was achieved with tomato pomace as agroindustrial residue corresponding to the 14th day of culture. Based on these results *C. versicolor* was cultivated in a basal medium plus tomato pomace in a stirred bioreactor.

Endocellular and exocellular protein-bound polysaccharides were quantified. The concentration of the polysaccharide compounds was higher in the supernatant than in mycelia and supernatant complex has higher protein content. The main protein-bound polysaccharides produced by *C. versicolor* ranged between molecular weights of 1.3×10^3-8.9×10^4 Da.

The comparison of the results obtained in this study with those reported in the literature, let us to confirm the interest of this selected culture medium with tomato pomace, in order to maximise the production of complexes protein-polysaccharides by *C. versicolor*. Besides, this clean process allows valuing the agro-industrial residues with a low cost and a higher production of polysaccharide compounds.

PRODUCTION, PURIFICATION AND PARTIAL CHARACTERIZATION OF PROTEIN – BOUND POLYSACCHARIDES FROM Pleurotus ostreatus AND Lentinula edodes

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Publicado em:
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The medicinal power and the nutritional value of some mushrooms are widely known. However, only in the last decades of the last century that it was possible to isolate and partially characterize some biologically active anti-cancer substances.

The therapeutic properties of mushrooms are attributed mainly to their polysaccharide content which has exhibited immunomodulatory properties such as anti-cancer, anti-viral and anti-bacterial activities. Protein-bound polysaccharides are macromolecules which consist of a central core protein to which are attached a number of polysaccharide chains and PSP and PSK from *Coriolus versicolor* are the most widely studied protein-bound polysaccharides.

Although protein-bound polysaccharides from mushrooms exhibit important medicinal properties, there is little information in the literature about their biological and physico-chemical properties.

Therefore, the aim of this work consists of production, purification and partial characterization of these protein-bound polysaccharides from *Pleurotus ostreatus* and *Lentinula edodes*.

The fungal strains were grown in several culture media such as whey permeate supplemented with glucose, yeast extract and suitable salts. The cultures were grown in agitated and aerated bioreactors at pH 5.5 and 27°C, with pH and temperature control for 10 days and suitable daily samples were removed from the reactor. These samples were centrifuged and intracellular and extracellular protein-bound polysaccharides were extracted from the biomass and culture supernatant, respectively. Subsequently, these polysaccharides were purified by gel filtration chromatography on a Sephacryl S-300-HR column and fractions were analysed for protein, superoxide dismutase (SOD) activity and polysaccharides. Fractions containing protein-bound polysaccharides were characterized by HPLC which revealed UV and RI peaks with retention times of 6 and 13 min., respectively. On the other hand, FTIR analysis of these polysaccharide preparations revealed absorption peaks at 910, 989, 1078, 1644, 2335, 2363 and 3115 cm^{-1} which are characteristics of such macromolecules. Moreover, purified polysaccharides exhibited SOD activity which is in agreement with the data published in the literature.

The results presented strongly suggest that these basidiomycete strains produce high levels of free and protein-bound polysaccharides which exhibit similar physico-chemical properties compared with the data in the literature as far as HPLC and FTIR analysis are concerned.

STRUCTURAL AND KINETICS EFFECTS OF Pseudomonas aeruginosa WILD-TYPE AMIDASE ENCAPSULATION IN REVERSED MICELLES

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The present work involves the entrapment of either cell-free extract or whole cells from both *Pseudomonas aeruginosa* L10 and AI3 in a reversed micellar system composed of cationic surfactant tetradecyltrimethyl ammonium bromide (TTAB) in heptane/octanol (80/20%). The reaction used to study the effect of the encapsulation was a transamidation reaction catalysed by the enzyme amidase (E.C. 3.5.1.4) which isexpressed by both bacteria. The effect of micellar water content (wo) in the enzyme activity was also evaluated. The results demonstrated a major increase in the activity of acetohydroxamic acid synthesis in reverse micelles when compared with the conventional aqueous system. Furthermore when micelles water content was changed abell-shaped profile was obtained for amidase specific activity in both cell-free extract and whole cells with a maximum activity exhibited at ωo =10. The study of storage stability of whole cell and cell free extract when entrapped in reverse micelles at 24°C revealed a half-life of respectively 17 days and 26 days for *Pseudomonas aeruginosa* AI3 strain and11 days and 8.5 days for *Pseudomonas aeruginosa* L10.

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CATALYTIC CARACTERIZATION OF PILLARED CLAYS THROUGH TOLUENE METHYLATION REACTION

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Proceedings em CD do 5º Congresso Luso-Moçambicano de Engenharia, Simpósio de Catálise e Processos Catalíticos CLME'2008, Maputo, 1 a 3 de Setembro de 2008.

Pillared clays (PILCs) with Al and Zr oxide pillars, obtained from a natural Portuguese montmorillonite from Porto Santo (PTS) were studied in terms of their structure (from X-ray diffraction patterns) and texture (N_2 adsorption).The catalytic properties of the samples were assessed through toluene methylation reaction. As comparison material a commercial zeolite HZSM-5 (Si/Al=19) was used. The toluene conversion at short time on stream (2 min) over PILCs, although smaller than the value obtained with HZSM-5, attains values of 37 (molar %). In all cases the reaction products are a mixture of xylenes, ethyltoluenes and trimethylbenzenes isomers. Over all samples, xylenes are the greater and primary products. Ethyltoluene isomers are the minor products over HZSM-5 and Al-PTS. In the case of Zr-PTS the percentage of these isomers is substantially higher and almost the same as for trimethylbenzenes.

A DYNAMIC MODEL FOR THE DE-ABSORPTION OF CARBON DIOXIDE FROM MONOETHANOLAMINE SOLUTION

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Due to the adverse effect of CO_2 from fossil fuel combustion on the earth's ecosystems, the most cost effective method for CO_2 capture is an important area of research. The predominant process for CO_2 capture currently employed by industry is chemical absorption in amine solutions. A dynamic model for the de-absorption process was developed with Monoethanolamine solution. Henry's law was used for modeling the vapour phase equilibrium of the CO_2, and fugacity ratios calculated by the Peng Robinson EOS were used for H_2O, MEA, N_2 and O_2. Chemical reactions between CO_2 and MEA were included in the model along with the enhancement factor for chemical absorption. Liquid and vapor energy balances were developed to calculate the liquid and vapour temperature, respectively. The model results compare favourably with other published results.

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Proceedings SIMS 2008, Oslo, Noruega.

DESENVOLVIMENTO DE CATALISADORES HETEROGÉNEOS PARA A TRANSESTERIFICAÇÃO DE TRIGLICÉRIDOS EM BIODIESEL

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Publicado em:
Proceedings em CD da 10ª Conferência Científica e Internacional em Engenharia Química e Biológica CHEMPOR2008, Braga, 4 a 6 de Setembro de 2008.

Biofuels are all fuel substances produced from Biomass which includes Biodiesel (single alkyl ester of fatty acids), Bioethanol and Biogas (mixture of Methane and CO_2). The highway transports activity, in a global level, is 98% oil dependent. In the EU, this activity is responsible by more than 20% of total CO_2 emissions and, more than 50% of these emissions concerns to the individual transport, which increase 22% since 1999. The climate changes, the increase of crude prices and the supply energetic security leads to the growing interest about biofuels potential as substitutes of oil fuels, like gasoline's and diesel. Nowadays, biodiesel is obtained essentially, from oleaginous plants by the transesterification process, which involves, as reactants, alcohol, essentially, methanol and a catalyst, preferably alkaline, liquid phase (NaOH, KOH, sodium methoxide). This process occurs with homogeneous catalysis. The main raw materials, which include the previously mentioned oils from oleaginous plants are, mainly Colza, Sunflower and SoyBean. It can be obtained, also, from other plants, such Palm. Chemically, biodiesel is described as a mixture of methyl ester's of fatty acids, where, through the transesterification process, are produced those ester's (single, double and triple triglycerides), and produces also, Glycerine as co-product reaction. The transesterification reaction is considered as the process with more technical effectiveness and with higher efficiency for biodiesel production in large scale, with minimization of by-products.

DESENVOLVIMENTO DE CATALISADORES HETEROGÉNEOS PARA A TRANSESTERIFICAÇÃO DE TRIGLICÉRIDOS EM BIODIESEL

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This study concerns the use of heterogeneous catalysts for biodiesel production, in order to replace the conventional homogeneous alkalines or acids catalysts, to eliminate the difficulties found in the current biodiesel/catalyst separation.

These new catalysts are solid, and they consist of an alternative and innovative solution in biodiesel production, allowing, more economic rentability and competitiveness to the process bringing, more environmental compatibility, when compared with the conventional processes. In fact, the use of heterogeneous catalytic systems in the transesterification of triglycerides implies the elimination of several washing/recovery biodiesel/catalyst process steps, in order to ensure a higher efficiency and rentability of the process, lowering the production costs. There is, also, the strong possibility of being implemented in a continuous way, with the construction of a fixed bed catalytic reactor. The utilisation of heterogeneous catalysts implies higher lifetimes, as there is no need to perform their recirculation to the initial step (mixture), since catalyst utilisation time is higher than the homogeneous catalytic processes. This means less catalyst replacements on the fixed bed catalytic reactor, which leads to a higher quality of the final product and, also, to the by-product, glycerine.

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Proceedings em CD da 10ª Conferência Científica e Internacional em Engenharia Química e Biológica CHEMPOR2008, Braga, 4 a 6 de Setembro de 2008.

DYNAMIC SIMULATION OF CO_2 ABSORPTION FROM POST COMBUSTION GASES

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Proceedings em CD da 10ª Conferência Científica e Internacional em Engenharia Química e Biológica CHEMPOR2008, Braga, 4 a 6 de Setembro de 2008.

CO_2 capture from combustion flue gases is currently an issue of main interest due to the high taxes being imposed on industrial companies as a measure to achieve CO_2 emissions abatement. CO_2 capture can be efficiently achieved by gas absorption using amines, namely Monoethanolamine (MEA). Based on henrys law, validated with previously published experimental work, this study considers the development of a dynamic model of an absorption column for post combustion CO_2 capture. A dynamic model of the temperature swing de-absorption process was developed with the integration of both models for absorption and de-absorption (with the introduction of heat exchangers, pumps and other ancillary equipment). A control system for the process was also devised, comprising the pertinent sensors, and various control structures for the absorption column were tested and compared, such as single loop PID controllers (including the pairing problem) and MPC.

HIDROISOMERIZAÇÃO DE N-HEXANO SOBRE CATALISADORES COMPÓSITOS À BASE DE ZEÓLITOS E MATERIAIS MESOPOROSOS

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Neste trabalho estudou-se o comportamento de catalisadores compósitos na reacção de hidroisomerização de n-hexano. Os materiais são constituídos pelo zeólito BEA na forma ácida e por materias mesoporosos – Al/SBA-15, Al/MCM-41 ou uma argila porosa heterostrutural PCH – impregnados com Pt e preparados por mistura mecânica. O desempenho catalítico dos compósitos foi comparado com o dos materais constituintes, impregnados com Pt.
A adsorção de N_2 a -196ºC sobre todas as amostras mostra que a presença de Pt não afecta significativamente a porosidade dos materiais, indicando ainda que a Pt se encontra dispersa mioritariamente na superfície externa. Na reacção de hidroisomerização de n-hexano apenas no compósito Pt-PCH+HBEA se observa um efeito sinergístico que traduz num ligeiro aumento da selectividade em produtos bi-ramificados, quando comparado com o catalisador Pt-HBEA.

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Actas do XXI Simposio Iberoamericano de Catalisis (SICAT 2008) Málaga, Espanha, 2008, Edição em CD-Rom.

INFLUÊNCIA DE ELEMENTOS DE TERRAS RARAS EM CATALISADORES BIFUNCIONAIS À BASE DE ZEÓLITO BEA NA REACÇÃO DE HIDROISOMERIZAÇÃO DE N-HEXANO

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Publicado em:
Actas do XXI Simposio Iberoamericano de Catalisis (SICAT 2008) Málaga, Espanha, 2008, Edição em CD-Rom.

Neste trabalho estudou-se o comportamento de catalisadores Pt/BEA, contendo elementos de terras raras (TR), na hidroisomerização de n-hexano. Os elementos de TR e a Pt foram introduzidos no zeólito HBEA por permuta iónica. A função metálica dos catalisadores foi caracterizada por quimisorção de H_2 e pela reaccção modelo de hidrogenação do tolueno. Os dados da caracterização do metal mostram que a presença de TR provoca modificações nas propriedades electrónicas da Pt o que se traduz por um aumento na actividade hidrogenate e dispersão metálica. Na hidroisomerização de n-hexano a presença de teores em TR inferiores a 1% (em massa) traduz-se por um ligeiro aumento na selectividade aos produtos bi-ramificados. Este efeito perde-se à medida que os teores em TR aumentam, devido à formação de óxidos de TR na vizinhança dos centros metálicos o que, por um lado, inibe o efeito nas propriedades hidrogenantes e, por outro lado, dificulta o acesso dos intermediários reaccionais aos centros metálicos.

MODIFICATION OF ZEOLITE POROSITY BY ALKALINE TREATMENTS

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In this work a set of MOR, BEA, MFI and FER zeolites were submitted to alkaline treatment in order to extract silicon from the framework, resulting in the generation of mesoporosity inside the zeolite crystals. The samples where characterized by X-ray powder diffraction and scanning electron microscopy. The textural properties were studied by N_2 adsorption at low temperature. The effect of the desilication treatment on the acidity was evaluated by the model reaction of catalytic craking of n-heptane and by pyridine adsorption followed by infrared spectroscopy.

Publicado em:
Actas do 10th Chemical and Biological Engineering Conference (CHEMPOR 2008), Braga Portugal 2008, Edição em Cd-ROM.

OPTIMIZATION OF HYDROXAPATITE SYNTHESIS

Gomes, J.F.[1,2]; Granadeiro, C.[1]; Silva, M.[1]; Hoyos, M.[1]; Silva, R.[1]; Antunes, F.[1]; Amaral, J.[1]; Vieira, T.[3]

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Publicado em:
Proceedings em CD da 10ª Conferência Científica e Internacional em Engenharia Química e Biológica CHEMPOR2008, Braga, 4 a 6 de Setembro de 2008.

Hydroxyapatite (HAP) 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 work performed regarding the synthesis of this compound by a wet method comprising the direct precipitation of orthophosphoric acid solution and a calcium hydroxide solution. The 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 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.

PREPARATION OF MESOPOROUS CARBONS USING A POROUS CLAY HETEROSTRUCTURED AS TEMPLATE

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In this work two mesoporous carbon replicas were prepared using a porous clay heterostructure - obtained from a Portuguese natural mot-morillonite - as template and furfuryl alcohol as carbon source. The samples where characterized by X-ray powder diffraction, scanning electron microscopy and N2 adsorption at low temperature. The ash content and the pH at the point of zero charge were also determined. The previous acidification of the surface revealed to be not important since the samples prepared with and without the previous impregna-tion with p-toluenesulfonic acid presented the same textural, structu-ral and morphological characteristics. The surface chemistry properties must also be similar since the carbons present the same pH at the point of zero charge.

Publicado em:
Actas do 10th Chemical and Biological Engineering Conference (CHEMPOR 2008), Braga Portugal 2008, Edição em Cd-ROM.

NOME INFLUENCE OF THE REACTOR CONTENTS RECIRCULATION ON METHANE PRODUCTION – ANAEROBIC DIGESTION OF FRUITS, VEGETABLES AND GRASS WASTE FEEDSTOCKS

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Publicado em:
Proceedings da Chempor 2008 - 10th International Chemical Engineering Conference, Braga, 4 a 6 de Setembro de 2008, (PC-085).

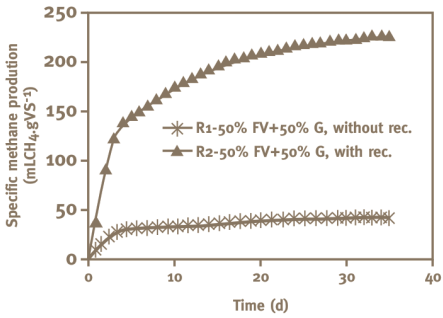
Anaerobic digestion process generates two main products: biogas, a mixture of methane and carbon dioxide, and compost. In Europe, the study of anaerobic digestion of solid wastes only started in the 1980's (Mata-Alvarez, 2002). After the energy crises of the 1970's and the global environmental considerations, such as greenhouse effect, anaerobic digestion process had a significant development, because this waste treatment produce a renewable energy source, limiting the biogas emissions that cause adverse effects and also permit organic mater and nutrients recovery, with the application of compost in soil. Another benefit associated with the anaerobic digestion is the possibility to reduce the amount of waste sent to landfill, which is a goal expressed in European Directive 1999/31/CE.

Fruits and vegetables wastes represent potential resource energy (Gunaseelan *et al.*, 2004). This kind of waste is produced in great quantity from markets, restaurants, agriculture and others domestic activities. Also grass is a waste produced in significant quantities from golf clubs, stadiums and gardens.

In Portugal, the first waste anaerobic digestion plant was constructed only in the last years. In order to fully evaluate the overall anaerobic digestion process, particular attention should be devoted to the study of specific waste characteristics and process parameters. In fact, the ability to manage a biological process is deeply related to substrate biodegradability and proper control conditions of the process. Adverse effects to the overall digestion process may sometimes occur when poorly characterized wastes one added to a stable processing reactor, or used in conjunction with another type of waste (Misi and Forster, 2001).

The objective of this study was to determine the influence of recirculation of the digestion mixture on methane production from anaerobic digestion of fruits, vegetables and grass. The mixture used contains 50% of fruits and vegetables and 50% of grass. This mixture was selected from previous studies carried out with a wide range of fruits and vegetables to grass ratios, as the one that yield a higher methane production.

The experiments were made with two batch reactors with 10L capacity each, using an incubation period of 35 days at a mesophilic range. One of the reactor worked without recirculation (R1) and the other with recirculation of the contents (R2).
During the experiment, the biogas volume and its composition were monitored for each reactor. The liquid phase was also analysed for COD, pH, TS, VS and volatile fatty acid determination.
The methane production for both reactors is show in Figure 1. Maximum specific methane production was achieved in 5 day for R1 and in 15 days for R2. R2 presents a greater methane production (223.24 mL $CH_4 \bullet g^{-1}VS$) than R1. The average of methane percentage in the biogas produced was 45% and 70% for R1 and R2 respectively.
In both reactors, and during all the period of incubation, the pH of the digestion mixture do not need to be adjusted externally, since it was found that it remains in the adequate range for anaerobic digestion (Table 1).



Reactor	pH initial	pH final	Maximum specific methane production (mL $CH_4 \bullet g^{-1}VS$)
R1	7.42	7.38	41.54
R2	7.65	7.49	223.24

Table 1. pH and maximum specific methane production for R1 and R2

The overall volume of methane produced was much larger in R2 than R1. This is probably due to the recirculation system which ensures a good homogenization of the reactor contents. Similar results were presented by Sponza and Agdag (2004).

OPTIMIZATION OF HYDROXAPATITE SYNTHESIS

Gomes, J.F.[1,2]; Granadeiro, C.[1]; Silva, M.[1]; Hoyos, M.[1]; Silva, R.[1]; Antunes, F.[1]; Amaral, J.[1]; Vieira, T.[3]

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Publicado em:
Proceedings em CD do 5º Congresso Luso-Moçambicano de Engenharia, Simpósio de Catálise e Processos Catalíticos CLME'2008, Maputo, 1 a 3 de Setembro de 2008.

Hydroxyapatite (HAP) 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 work performed regarding the synthesis of this compound by a wet method comprising the direct precipitation of orthophosphoric acid solution and a calcium hydroxide solution. The 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 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.

PESQUISA DE NOVOS CATALISADORES SÓLIDOS PARA A PRODUÇÃO DE BIODIESEL

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Neste artigo, os autores pretenderam mostrar alternativas mais rentáveis do ponto de vista económico e mais sustentáveis para a produção de Biodiesel, com catalisadores heterogéneos, em alternativa ao uso dos catalisadores convencionais homogéneos alcalinos, na reacção de transesterificação, como o hidróxido de sódio ou o metilato de sódio. Este documento resulta de um trabalho experimental de doutoramento, elaborado pelo autor correspondente deste artigo, o qual pretende desenvolver e optimizar um novo processo de produção de Biodiesel com recurso a catalisadores sólidos, capaz de produzir o biocombustível de maneira contínua, sem interrupções. A optimização deste processo possui muitas diferenças relativamente ao actual processo com catalisadores homogéneos. A principal vantagem está relacionada com o facto de os custos de investimento, nomeadamente de produção, serem significativamente menores com catálise heterogénea, porque não são necessárias as etapas de separação/recuperação do catalisador no Metanol, na fase de Biodiesel e na fase de Glicerina. Neste artigo, está também descrita uma revisão da pesquisa bibliográfica já realizada. Finalmente, os autores pretendem mostrar as principais conclusões relativas aos parâmetros de optimização mais adequados do referido processo, como temperatura reaccional, ratio metanol/óleo vegetal e ratio catalisador/óleo, tempo de reacção e propriedades do catalisador. Uma proposta de *flow-sheet* deste processo de produção é também apresentada.

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Proceedings em CD da Conferência Científica e Internacional Bioenergy: Challenges and Opportunities, Guimarães, 6 a 9 de Abril de 2008.

STUDIES ON THE DEVELOPMENT OF HETEROGENEOUS CATALYSTS FOR TRANSESTERIFICATION OF TRIGLYCERIDES

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Publicado em:
Proceedings em CD do 5º Congresso Luso-Moçambicano de Engenharia, Simpósio de Catálise e Processos Catalíticos CLME'2008, Maputo, 1 a 3 de Setembro de 2008.

This paper describes preliminary work done by the authors towards the development of new metallic heterogeneous catalysts that are to be used in the trans-esterification reaction of triglycerides, which is of considerable interest in the production of biodiesel. Biodiesel, is a mixture of mono-alkyl esters of fatty acids, and is currently manufactured by trans-esterification of triglycerides with methanol using NaOH or KOH as liquid base catalyst. Catalysts as such are corrosive to the equipment and another drawback is that these catalysts are in liquid phase and must be neutralized after the completion of the reaction, typically using HCl, thus producing salt streams. Moreover, due to the presence of free fatty acids it reacts to form soaps as unwanted by--products, hence requiring more expensive separation processes. Therefore, there is a great need on the development of industrial processes for biodiesel production using solid acid catalysts. The key benefit of using solid acid catalysts is that no polluting by-products are formed and the catalysts do not have to be removed since they do not mix with the biodiesel product.

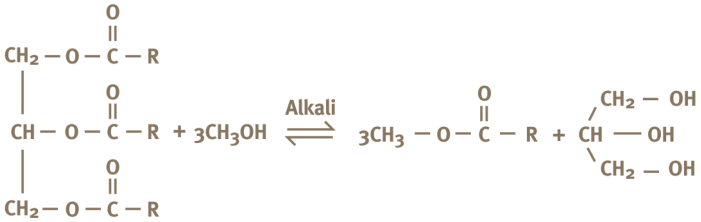

Figure 1. Transesterification reaction for biodiesel production.

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SUPERCRITICAL FLUID EXTRACTION OF COMPOUNDS FROM CORIANDER SEEDS: EXPERIMENTS AND MODELLING

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Supercritical fluid extraction of the volatile and non-volatile fractions from coriander seeds was carried out under different conditions of pressure (90, 100 and 250bar), temperature (40 and 50ºC), mean particle size (0.4, 0.6 and 0.8 mm) and CO_2 flow rate ($2.19x10^{-4}$, $3.05x10^{-4}$ and $4.54x10^{-4}$kg/s) to understand the influence of the process parameters on the composition and extraction yield of the oil fractions. The best extraction conditions for volatile oil were at 90bar, 40ºC, 0.6 mm and $3.05x10^{-4}$kg/s and for the non-volatile oil 250bar, 40ºC, 0.6 mm and $3.05x10^{-4}$kg/s (after the removal of the volatile oil).
A model based on the concept of broken and intact cells was applied to the supercritical CO_2 extraction of the volatile oil. A good agreement was obtained between the model and our experimental measurements. Moreover, a comparative evaluation of the antioxidant activity of the SFE extracts, of the essential oil (Hydrodistillation) and Soxhlet extract obtained with pentane, after deodorization, was performed using the 2,2-diphenyl-1-picrylhydrazyl method (DPPH).

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Proceedings of the 11th European Meeting on Supercritical Fluids, Barcelona, (Spain), 4-7 Maio de 2008, pp. 1-4.

04

SÍNTESE E CARACTERIZAÇÃO DE COMPLEXOS DE FERRO(II) E RUTÉNIO(II) COM LIGANDOS NITRILO E ACETILETO: POTENCIAIS FIOS MOLECULARES?

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Publicado em:
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Os compostos envolvendo unidades bimetálicas de valência mista ou grupos organometálicos ligados através de sistemas orgânicos conjugados podem ser utilizados como fios moleculares na área da electrónica molecular ou como componentes optoelectrónicos.

Os fios moleculares envolvendo centros metálicos podem ser constituídos por um sistema orgânico deslocalizado que estabelece a ponte entre os centros metálicos terminais, sendo ambas as partes responsáveis pelo desempenho final do fio molecular. Os espaçadores orgânicos são responsáveis pelas propriedades electrónicas e pelo comprimento do fio; enquanto que os centros metálicos, ao introduzirem electrões no sistema, aumentam a condutividade.

Os ligandos nitrilo e acetileto têm sido extensamente utilizados na síntese de complexos de metais de transição electronicamente ricos e com uma extensa conjugação π. A sua contribuição tem sido igualmente útil na construção de fios moleculares envolvendo complexos bimetálicos, na medida em que permitem a comunicação electrónica entre fragmentos metálicos terminais através das ligações deslocalizadas.

Nesta comunicação apresentaremos, a síntese de diversos complexos de ferro(II) e ruténio(II) com ligandos nitrilo e acetileto baseados em diferentes sistemas π deslocalizados, tais como o $N{\equiv}C\text{-}CH_2{-}C{\equiv}N$, $N{\equiv}C\text{-}C_6H_4{-}C{\equiv}N$, $N{\equiv}C\text{-}CH{=}CH\text{-}C{\equiv}N$ e $N{\equiv}C\text{-}C_6H_4\text{-}C{\equiv}CH$, e diferentes fragmentos metálicos $[CpFe(dppe)]^+$, $[CpRu(dppe)]^+$, $[CpFe(CO_2)]^+$, $[(Dppe)_2\ FeH]^+$, etc.. Os complexos obtidos foram caracterizados utilizando as técnicas espectroscópicas usuais: UV-VIS, IV e RMN. A eficiência da interacção electrónica entre os centros metálicos, ao longo dos sistemas π, foi avaliada por estudos electroquímicos (voltametria cíclica) e por análise de difracção de raios X em compostos seleccionados.

SYNTHESIS AND CHARACTERIZATION OF NOVEL OCTAHEDRAL $[FeH(DPPE)_2(NCR)][PF_6]$ COMPOUNDS

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Publicado em:
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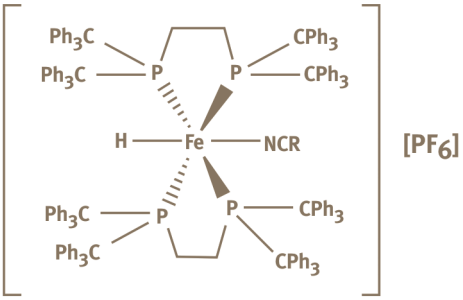
Organometallic compounds have been extensively studied in search of new materials with enhanced NLO properties due to their large hyper-polarizabilities, fast response times and architectural flexibility. Organometallic molecules with a highly polarisable π-conjugated backbone with an electron-donor (D) and an -acceptor (A) groups attached to opposite ends can a large second-order nonlinear susceptibility.
In the search of new systems, we synthesised iron(II) octahedral complexes with the general formula $[FeX(biphosphine)_2(NCR)](PF_6)$ (X=Cl, I or H; bisphosphine=DMPE, DPPE, dppen, odppb; NCR=mono- or dinitrobenzonitriles) with interesting results towards NLO properties.
In this communication, we report the synthesis and characterization of a series of $[FeH(DPPE)_2(NCR)][PF_6]$ derivatives. The acceptor capacity of the nitrile chromophore was changed due to the position (*ortho* and *para*) of the nitro group and with the change in length of the conjugated backbone. The results were analysed to evaluate the electronic richness of the metal centre and the influence of the structural changes of the coordinated nitrile, which may give some contribution to understand the relationships between structure and NLO responses.



MONOCYCLOPENTADIENYLRUTHENIUM COMPLEXES FOR SECOND-ORDER NLO PURPOSES

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Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, Química e Inovação, Porto, 11 - 13 de Junho de 2008.

Organometallic compounds have given rise to a great deal of interest owing to their application in the field of nonlinear opics (NLO). For second-order nonlinear optics (SONLO) strongly asymmetric systems are needed, which led to the development of typical push-pull systems in which the metal centre, bound to a highly polarizable conjugated backbone, acts as an electron releasing or withdrawing group. Among the organometallic compounds presenting this donor-π-system-acceptor feature, η^5-monocyclopentadienyliron and ruthenium moieties were found to be much more efficient donor groups for second-order NLO purposes than the traditional organic donor groups, leading to higher first hyperpolarizabilities (β). Recent results on η^5-monocyclopentadienyliron complexes presenting thiophene nitrile chromophores showed an enhanced SONLO performance when compared to that observed on analogue benzenoid structures. Also, the first hyperpolarizability of these complexes was found to be influenced by a compromise between the conjugation length of the chromophores and the metal-to-ligand charge-transfer.
I our continuous effort to understand the role played by the organometallic fragment on the SONLO properties and to establish detailed structure-NLO activity correlations, we now study a series of complexes of general formula $[RuCp(P\_\_P)(NC\{SC_4H_2\}nNO_2)][PF_6]$ (P__P=dppe, (+)-diop; n=1-3). Spectroscopic and electrochemical data will be used in order to evaluate the effect of the phosphine coligand and the length of the conjugated ligand on the second-order NLO response of the complexes. The results will be compared to those found in parent iron derivatives.

04

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

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The present study reports on the biotransformation of the azo dye Sudan Orange G by the oxidative bacterial enzyme CotA-laccase from *Bacillus subtilis*. In the absence of redox mediators over 98% of Sudan Orange G is decolorized within 7 hours. However the presence of catalytic amounts of 2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid) leads to a two-fold increase in the rate of biotransformation. Enzyme inhibition at high SOG concentrations was observed and a K_i value of 474 μM calculated. The redox potential of the SOG dye depends on pH as shown by cyclic voltammetry; E^o decreases with increasing pH values up to ≅ 7 and then remains constant. These results are consistent with the determined p_{Ka} values of 6.9 and 11.7, of the two oxidizable groups of SOG, and are in agreement with the bell-shape pH profile of the enzyme with an optimum of 8. Seven biotransformation products were identified using high-performance liquid chromatography and mass spectrometry. Furthermore, a mechanistic pathway for the azo dye conversion by CotA-laccase is proposed. Taken together, these approaches revealed that the enzymatic oxidation of the Sudan Orange G results in the production of oligomers and, possibly polymers, through radical coupling reactions. This correlates with the presence of low aqueous soluble products and the final brown color of enzymatic reactions. A bioassay based on the inhibitory effects over the growth of *Saccharomyces cerevisiae* shows that the enzymatic bioremediation process reduces 3-fold the toxicity of Sudan Orange G.

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04

COUPLING REACTIONS BETWEEN SUBSTITUTED AROMATIC AMINES USING BACTERIAL CotA-LACCASE AS BIOCATALYST

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The use of biocatalytic systems represents an important field in Green Chemistry as an alternative to conventional synthetic approaches. The interest in new sustainable processes based on the use of enzymes in organic synthesis has increased, because biochemical reactions are more attractive as alternative routes for the synthesis of fine chemicals. Increasing interest has been focused on the application of laccases (benzenediol:oxygen oxidoreductases E.C. 1.10.3.2), a large subfamily of multi-copper oxidases, which use the available molecular oxygen as the electron acceptor, as new biocatalysts in organic synthesis.

In this study we investigated the coupling reactions of substituted aromatic amines using the recombinant CotA-laccase, a bacterial enzyme from *Bacilius subtilis*, which have been extensively studied at the molecular level, as a biocatalyst. The laccase-mediated heteromolecular coupling reactions of several aromatic amines precursors (1,4-phenylenediamine, 4-nitroaniline, etc.) into coloured products, were performed under mild conditions (at 37°C in aqueous medium, for two pH values), followed by TLC and UV/Vis spectroscopy and the resulting products analyzed and characterized by IR and NMR spectroscopies.

Several parameters influencing the coupling reaction upon laccase catalysis were also tested, namely the substrate and enzyme concentrations, the reaction time, the oxygen pressure and the use of a biphasic system with an organic solvent as reaction medium.

SYNTHESIS OF HOMO AND HETEROBIMETALLIC SYSTEMS BASED ON NITRILE AND ALKYNYLIRON(II) AND RUTHENIUM(II) DERIVATIVES

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Molecular wires comprising homo or heterobimetallic units with redox-active organometallic groups connected by conjugated organic chains could be exploited in molecular electronics and optoelectronic devices. Nitrile and alkynyl ligands offer synthetic and structural versatility and the metal nitrile and acetylide linkages have proven to be useful to obtain rich complexes with extended π-conjugation. Therefore, they can be used in bimetallic molecular wires, allowing electronic communication between the terminal end groups through delocalized bonds. We report herein the synthesis of several iron(II) and ruthenium(II) nitrile and/or acetylide complexes based on organic spacers, such as $N{\equiv}C\text{-}CH_2\text{-}C{\equiv}N$, $N{\equiv}C\text{-}CH{=}CH\text{-}C{\equiv}N$ and $Y{\equiv}C\text{-}C_6H_4\text{-}C{\equiv}Y$ (Y=N or C) and different metallic fragments ($[CpM(dppe)]^+$ (M=Fe, Ru), $[CpFe(CO)_2]^+$, etc. For the complexes, spectroscopic (UV-Vis, IR and NMR) and electrochemical studies (cyclic voltammetry) were used to evaluate the efficiency of the electronic interaction between the metal centres along the bridging systems.

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Livros de Resumos da International Conference on Organometallic Chemistry-ICOMC 2008, Rennes, 13-18 de Julho de 2008.

BENZOYLDIAZENIDO-Re(III) AND OXO-Re(V) COMPLEXES BEARING N,N- AND N,O-TYPE LIGANDS

Furtado, A.[1]; Travassos, C.[1]; Kirillov, A.M.[2]; Guedes da Silva, M.F.C.[2,3]; Martins, L.M.D.R.S.[1,2]; Alegria, E.C.B.A.[1,2]; Pombeiro, A.J.L.[2]

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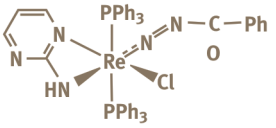
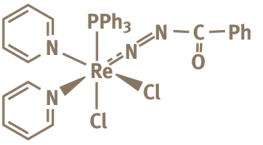
Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, Porto, 11 a 13 de Junho de 2008.

Recently, we have synthesized a series of Re(V), Re(III) and Re(I) complexes with various *N*-donor ligands (including scorpionates, aminopolyalcohols, aminoacids and *N*-heterocycle species), which have shown some interesting structural, catalytic and electrochemical features.

Extending these studies to other *N*-donor ligands such as 2-aminopyrimidine (2-NH_2-pyrm), 2,2'-bipyridine (2,2'-bpy) and pyrazinecarboxylic acid (Hpca), we now report the new benzoyldiazenido-Re(III) compounds [ReCl{η^1-NNC(O)Ph}(2-NH-pyrm)$(PPh_3)_2$] (**1**) and [$ReCl_2${η^1-NNC(O)Ph} (2,2'-bpy)(PPh_3)] (**2**), as well as oxo-Re(V) complex [$ReOCl_2$(pca)(PPh_3)] (**3**). They have been prepared by reacting the corresponding *N*-species with either benzoylhydrazido- [$ReCl_2${η^2-NNC(O)Ph}$(PPh_3)_2$] or oxo-rhenium [$ReOCl_3(PPh_3)_2$] precursors, and characterized by IR, ^{1}H, ^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectroscopies, FAB$^+$-MS, elemental and single-crystal X-ray diffraction (for **1** and **2**) analyses.



1



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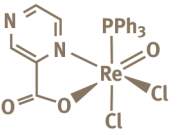

3

NEW RHENIUM(III) COMPLEXES BEARING WATER SOLUBLE LIGANDS

Lopes, G.J.O.C.[1]; Smolenski, P.[2]; Alegria, E.C.B.A.[1,2]; Martins,L.M.D.R.S.[1,2]; Pombeiro, A.J.L.[2]

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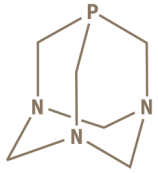
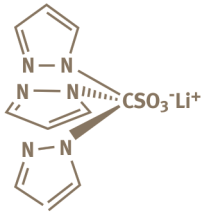
Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, Porto, 11 a 13 de Junho de 2008.

Within the expanding coordination chemistry of rhenium, the synthesis of complexes that are soluble in ambient friendly solvents, specially water, has not yet been significantly explored [1]. Thus, the application of hydro-soluble 1,3,5-triaza-7-phosphaadamantane (PTA), tris (pyrazolyl) methanesulfonate, $SO_3C(pz)_3^-$ (Tpms) and their derivatives as ligands would be particularly promising in view *e.g.* of the interesting catalytic, medicinal or photoluminescent properties of some complexes with such ligands.



PTA



Tpms

Herein we report the synthesis of new water-soluble rhenium (III) complexes bearing PTA, *e.g.* $[ReCl_2(N_2COPh)(PTA)_3]$, or the N_3 tripodal anionic tris(1-pyrazolyl)methanesulfonate $SO_3Cpz_3^-$ ligand.
The new complexes have been characterized by IR and multinuclear NMR or EPR spectroscopies, FAB-MS spectrometry and elemental analysis.

INVESTIGAÇÃO NOS ENSINOS SUPERIOR - SECUNDÁRIO: UMA EXPERIÊNCIA EM QUÍMICA INORGÂNICA

Pontinha, A.; Pacheco, V.; Martins, L.

Departamento de Engenharia Química, ISEL, Lisboa, Portugal

Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, Porto, 11 a 13 de Junho de 2008.

Com o propósito de contribuir para o desenvolvimento e divulgação, no ensino secundário, das actividades de I&D realizadas no Laboratório de Química Inorgânica do Departamento de Engenharia Química do Instituto Superior de Engenharia de Lisboa, e motivar os alunos para a investigação e tecnologias associadas, realizaram-se vários estágios no âmbito da Ocupação Cientifica de Jovens nas Férias promovidos pela Agência Nacional para a Cultura Cientifica e Tecnológica - Ciência Viva.
Os trabalhos efectuados tiveram como objectivo preparar os alunos para a utilização de técnicas e equipamentos mais usados no Laboratório de Química Inorgânica, bem como promover o contacto entre os alunos do ensino secundário e os investigadores e professores da instituição.
Nesta comunicação são divulgados os referidos estágios, bem como a contribuição destas acções para a formação dos alunos.

PEROXIDATIVE OXIDATION OF CYCLOHEXANE IN WATER CATALYZED BY A CHLORO-SCORPIONATE IRON(II) COMPLEX

Martins, L.M.D.R.S.[1,2]; Alegria, E.C.B.[1,2]; Pombeiro, A.J.L.[2]

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The use of water as solvent in organic and organometallic chemical processes is a subject of current environmental, industrial and biological significance.

In pursuit of our interest on the functionalization reactions of saturated hydrocarbons, in particular oxidations, towards the development of methods for the use of such unreactive compounds as raw materials for organic syntheses, we have been able to synthesise and characterize half-sandwich complexes bearing the N_3 tripodal ligands hydrotris(1-pyrazolyl)methane ($HCpz_3$, Tpm) and tris(1-pyrazolyl)methanesulfonate ($SO_3Cpz_3^-$,Tpms), *e.g.*, $[MCl_n\{XC(pz)_3\}]^y$ (M = Fe, V or Cu; n=1-3; y = 0 or -1; X = H, SO_3) and found that they act as catalysts in the peroxidative oxidation of cyclohexane.

Of particular relevance for the establishment of a "green" process the ability of the hydro-soluble chloro-scorpionate iron(II) complex $[FeCl_2\{HC(pz)_3\}]$ to catalyze the oxidation of cyclohexane to cyclohexanol and cyclohexanone in water (without the need to add any organic solvent), with an overall turnover number (TON) of *ca.* 100.

Publicado em:
Livros de Resumos da XXIII International Conference on Organometallic Chemistry, Rennes, 13 a 18 de Julho de 2008.

VANADIUM CATALYSTS FOR THE PARTIAL OXIDATION OF ALKANES UNDER MILD CONDITIONS

Pombeiro, A.J.L.; Silva, T.F.S.; Mishra, G.S.; Kirillova, M.V.; Alegria, E.C.B.A.; Martins, L.M.D.R.S.; Kirillov, A.M.; Guedes da Silva, M.F.C.; Kuznetsov, M.L.; Palavra, A.; Silva, J.A.L. da; Fraústo da Silva, J.J.R.

Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, TU Lisbon, Lisboa, Portugal

Publicado em:
Livros de Resumos do 6th International Vanadium Symposium, Lisboa, 17 a 19 de Julho de 2008.

Partial oxidation reactions of saturated hydrocarbons under mild conditions are expected to provide promising methods towards the use of such unreactive compounds as raw materials for organic syntheses. This general aim constitutes a challenge to modern Chemistry and the field is also of biological significance in view of the ability of a few enzymes to catalyse the partial oxidation of alkanes.

Our initial studies by using, as a catalyst, Amavadin, a natural bare vanadium complex with a still unknown biological role, have been extended to other vanadium catalysts which are shown to be particularly active for the following general types of oxidation reactions:

| Peroxidative oxidations of alkanes to alcohols and ketones, typically with aqueous hydrogen peroxide (a “green” oxidant), at room temperature.

| Oxidations of alkanes with dioxygen (the ideal oxidant) in solvent free systems, by using supported catalysts on modified silica.

| Such reactions will also be compared with alkane carboxylations leading to carboxylic acids.

Some of the V-systems provide the highest catalytic activity so far reported in the field of alkane functionalization under mild or moderate conditions. They are compared with those based on other metals, and plausible radical mechanisms are discussed on the basis of radical trap and ^{13}C-labelled experiments, and of DFT theoretical studies.

NEW C-FUNCTIONALIZED TRIS (PYRAZOLYL)METHANES AND THEIR VANADIUM COMPLEXES

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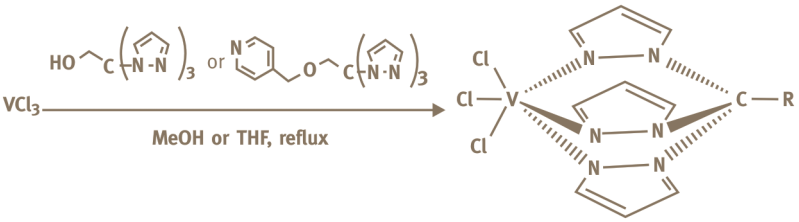
Publicado em:
Livros de Resumos do 6th International Vanadium Symposium, Lisboa, 17 a 19 de Julho de 2008.

Recently, we have initiated the study of the coordination chemistry of hydrotris(1-pyrazolyl)methane, $HC(pz)_3$ (pz = pyrazolyl), and its derivatives bearing substituents on the pyrazolyl rings (*e.g.*, hydrotris(3,5-dimethyl-1-pyrazolyl)methane, $HC(3,5\text{-}Me_2pz)_3$) or the C- methine carbon-substituted tris(1-pyrazolyl)methanesulfonate (as its lithium salt $Li[SO_3C(pz)_3]$), towards V, Fe, Cu or Re centres.[1-5] In addition, we have found that some of the synthesized scorpionate complexes of those metals can act as selective catalysts in the single-pot oxidation of ethane to acetic acid and in the peroxidative oxidation of cyclohexane to cyclohexanol and cyclohexanone.

Herein we report the study of the reactivity of hydrotris(1-pyrazolyl) methane towards the methine carbon functionalization and the coordination of the obtained C-functionalized scorpionates to a V centre. Hence we have prepared C-functionalized tris(pyrazolyl)methane derivatives $RC(pz)_3$, R= CH_2OH or new $CH_2OCH_2(py)$ (py = pyridyl ring), and investigated their behavior at vanadium(III) centres:



R= $HOCH_2$ or $pyCH_2OCH_2$

The synthesis and characterization of the new scorpionate and V-complexes are reported.

04

MOLECULAR ELECTROCHEMISTRY OF TRANSITION METAL COMPLEXES BEARING SCORPIONATES AND OTHER NITROGEN-DONOR LIGANDS

Martins, L.M.D.R.S.[1,2]

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Publicado em:
Livros de Resumos do XV Encontro da Sociedade Portuguesa de Electroquímica, Lisboa, 3 a 6 de Setembro de 2008.

The coordination chemistry of nitrogen donor ligands, in particular the N_3 tripodal "scorpionate" ones Fig. 1), has been widely developed in the last years and their complexes have found applications in processes with biological and industrial significance.[1]
However, in spite of their relevance, scorpionate complexes have not yet been the object of an electrochemical investigation.
In pursuit of our interest on the coordination chemistry of N- and O-donor ligands,[2] including the scorpionate-type tris(1-pyrazolyl) methane, towards transition metal centres (*e.g.* V, Fe, Cu, Mo, Ru or Re), we have recently focused our attention on the electrochemical behaviour of such types of complexes.
In this work, we present an overall view of the electrochemical properties of the above complexes, studied by cyclic voltammetry and controlled potential electrolysis in aprotic media, at room temperature, using Pt electrodes.
For some ligands, said electrochemical study has allowed to estimate, for the first time, their P_L and E_L ligand parameters which are of particular significance towards the understanding of the their electron donor/acceptor properties.
The obtained electrochemical results are discussed in terms of electron richness of the metal centres and the electronic properties of the chelating *N*-ligands, and compared with our previous electrochemical studies on related compounds.

ELECTROCHEMICAL BEHAVIOUR OF BENZOYLDIAZENIDO-Re(III) AND OXO-Re(V) COMPLEXES BEARING N,N- AND N,O-TYPE LIGANDS

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2 C. de Química Estrutural, Complexo I, Instituto Superior Técnico, TU Lisbon, Lisboa, Portugal

In pursuit of our interest on the coordination chemistry of rhenium, namely with *N*-donor ligands such as scorpionates,[1–3] aminopolyalcohols, aminoacids and *N*-heterocycle species,[4–7] we have extended these studies to the synthesis of new benzoyldiazenido-Re(III) compounds [ReCl{η^1-NNC(O)Ph}(2-NH-pyrm)(PPh_3)$_2$] (**1**) and [$ReCl_2${η^1-NNC(O)Ph}(2,2'-bpy)(PPh_3)] (**2**), as well as oxo-Re(V) complex [$ReOCl_2$(pca)(PPh3)] (**3**), derived from 2-aminopyrimidine (2-NH_2-pyrm), 2,2'-bipyridine (2,2'-bpy) and pyrazinecarboxylic acid (Hpca), respectively.

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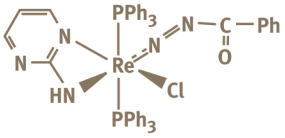

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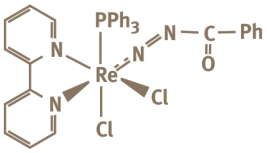

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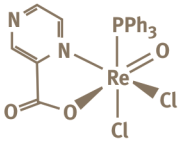

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In this work, we present the electrochemical behaviour of compounds **1**–**3**, investigated by cyclic voltammetry (CV) and controlled potential electrolysis (CPE), at a Pt electrode, in 0.2 M [^{n}Bu$_4$N][BF_4]/CH_2Cl_2 solution. The obtained electrochemical results are discussed in terms of electron richness of the Re(III or V) centres and the electronic properties of the chelating *N,N*- or *N,O*-ligands, and compared with our previous electrochemical studies on related compounds.[2–5]

COORDINATION POLYMERS BASED ON THETRIANGULAR [Cu3(μ3-OH) (μ-pz)3]$^{2+}$ CORE AND UNSATURATED CARBOXYLATES. CRYSTAL STRUCTURES, ELECTROCHEMICAL BEHAVIOR AND CATALYTIC ACTIVITY IN PEROXIDATIVE OXIDATION OF CYCLOALKANES

Garau, F.[1]; Pandolfo, L.[1]; Di Nicola, C.[2]; Ngoune, J.[2]; Pettinari, C.[2]; Monari, Magda[3]; Pombeiro, A.J.L.[4]; Martins, L.M.D.R.S.[4]; Karabach, Y.Y.[4]

1 University of Padova, Padova, Italy
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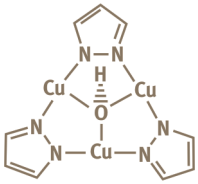
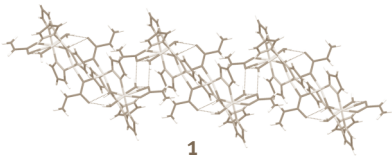
Livros de Resumos do 1st International Conference on Metal Organic Frameworks and Open Framework Compounds, Augsburg, 8 a 10 de Outubro de 2008.

In the last years the studies on 1D, 2D and 3D Metal Organic Frameworks (MOFs) have been continuously developed because these compounds present interesting properties and promising applications in numerous important fields, as gas storage, molecular recognition, catalysis, etc.,1 but this research field is far to be exhausted.
Recently, we developed a simple procedure to obtain trinuclear triangular copper(II) complexes, having the $[Cu_3(\mu_3\text{-OH})(\mu\text{-pz})_3]^{2+}$ core, (pz = pyrazolate) which charge is balanced by two carboxylate ions.[2] These neutral clusters behave as Secondary Building Units (SBUs) that self-assemble through carboxylate bridges and/or H-bonds to form different kinds of MOFs[2a,b] that resulted particularly active as catalysts for the peroxydative oxidation of cycloalkanes.[2c,3] It was possible also to exchange, partly or completely, the carboxylate ions with Cl^{-}[4] and with other anions (SO_4^{2-}, ClO_4^{-}, CF_3COO^{-}, $CF_3SO_3^{-}$, NO_3^{-})[5] obtaining different MOFs, all maintaining the $[Cu_3(\mu_3\text{-OH})(\mu\text{-pz})_3]^{2+}$ core.



Here we report the synthesis and the complete characterization of three different Cu(II) trinuclear triangular SBUs, 1-3, obtained by reacting Hpz and copper(II) unsaturated carboxylate (namely acrylate and methacrylate) in protic solvents (water, methanol).



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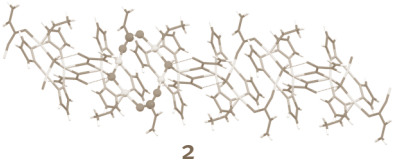

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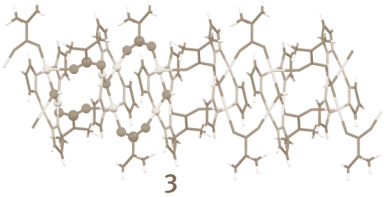

3

These SBUs self-assemble forming different 1D and 2D MOFs that catalyze the peroxydative oxidation of cycloalkanes. Moreover, the electrochemical behaviour of these compounds will be also illustrated.

QUIMICA E BIOLOGIA NA COZINHA: UM CONTRIBUTO PARA O ENSINO EXPERIMENTAL DAS CIÊNCIAS NO ENSINO SECUNDÁRIO

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2 Centro de Estudos de Engenharia Química, ISEL, Lisboa, Portugal

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O ensino experimental das ciências constitui uma importante meta que se encontra patente em todos os programas das disciplinas de Física, Química e Biologia do ensino básico e secundário. Por outro lado, a experiência de ensino tem mostrado que o nível de motivação dos alunos é elevado quando se lhes propõe a realização de actividades experimentais que possam responder a problemas reais do quotidiano.

É neste contexto que o Projecto *Química e Biologia na cozinha*, apoiado pelo Programa Ciência Viva VI, se tem desenvolvido em trabalho colaborativo entre o Centro de Estudos de Engenharia Química do Instituto Superior de Engenharia de Lisboa e a Escola Secundária de Fonseca Benevides, instituições com larga tradição no ensino experimental das ciências.

O Projecto, dirigido a alunos do 11º e 12º anos do Curso Profissional de Técnico de Análise Laboratorial, iniciou-se em Janeiro de 2006 e encontra-se em fase de finalização. Este Projecto baseou-se em actividades experimentais realizadas pelos alunos nos laboratórios de Análise Instrumental do Departamento de Engenharia Química do ISEL no âmbito da análise de produtos alimentares. Assim, de acordo com os objectivos e conteúdos programáticos da disciplina de Análises Químicas foram seleccionadas e adaptadas actividades experimentais já desenvolvidas no ISEL. Após preparação prévia das actividades em sala de aula na Escola Secundária Fonseca Benevides, os alunos deslocaram-se ao ISEL onde realizaram o trabalho experimental em pequenos grupos e procederam ao respectivo tratamento de resultados cuja discussão e análise crítica foi, posteriormente, efectuada em sala de aula. Idênticas actividades experimentais foram, também, implementadas nos laboratórios de Química da Escola Secundária Fonseca Benevides com a colaboração dos alunos. Encontra-se em elaboração um caderno de protocolos das actividades experimentais realizadas, o qual constituirá um dos produtos finais do Projecto, a divulgar nos sites das Instituições participantes.

EXTRACÇÃO DE ANTIOXIDANTES EM BRÓCOLOS ATRAVÉS DE ULTRASSONS

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A avaliação da capacidade antioxidante de produtos naturais tem sido alvo de intensa pesquisa nos últimos anos. O interesse pelos compostos com propriedades antioxidantes deve-se ao facto de lhes serem reconhecidas importantes funções na conservação dos alimentos e na protecção da saúde.

Os frutos e vegetais são fontes de antioxidantes naturais entre os quais se destacam as vitaminas, carotenóides, flavonóides e outros polifenóis. O consumo frequente destes produtos, segundo os estudos epidemiológicos que têm sido realizados, contribui para uma redução significativa do risco de doenças coronárias e de desenvolvimento de cancro. Aliás, o *World Cancer Research Fund e o American Institute for Cancer Research* alertam, desde 1997, para as vantagens de uma dieta rica em frutas e legumes, recomendando a ingestão diária de pelo menos 400 a 800g destes produtos.

Com o objectivo de avaliar o efeito de diferentes tipos de processamento no teor em polifenóis e na actividade antioxidante de diversos legumes foram preparados extractos vegetais de brócolos, associando à técnica de extracção com solventes orgânicos uma sonda de ultrassons. Foram ensaiadas várias condições de extracção e analisada a influência de parâmetros como o tempo e a amplitude de sonicação, a composição do solvente e a massa de amostra no doseamento dos polifenóis e na determinação da actividade antioxidante dos extractos. O método de Folin-Ciocalteau foi utilizado para a determinação do teor em polifenóis e a actividade antioxidante dos extractos avaliada com base na capacidade de inibição de radicais de 1,1-difenil-2-picrilhidrazil (DPPH).

Os resultados permitiram comparar os diferentes métodos de extracção e selecionar as melhores condições de ensaio. A extracção em presença de ultrassons revelou ser mais promissora em termos de rendimento e tempo de preparação dos extractos.

OPTIMIZAÇÃO DE UM MÉTODO DE HPLC PARA DETERMINAÇÃO DE ADITIVOS ALIMENTARES

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2 Dept. de Alimentação e Nutrição, Instituto Nacional de Saúde Dr. Ricardo Jorge, Lisboa, Portugal

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Livro de Resumo do XXI Encontro da Sociedade Portuguesa de Química, Porto, 11 a 13 de Junho de 2008.

Os aditivos alimentares desempenham um papel vital na indústria alimentar moderna, sendo geralmente utilizados com o objectivo de manter a qualidade e as características dos géneros alimentícios.
Para garantir o consumo seguro de alimentos com aditivos, a União Europeia legisla a sua utilização, limitando o seu uso, estabelecendo doses diárias admissíveis e obrigando os Estados Membros a estabelecer um sistema regular de vigilância para monitorização do consumo. Para obter essa informação, para além de dados de consumo são também necessários métodos de análise robustos de modo a quantificar os níveis dessas substâncias numa larga variedade de matrizes alimentares.
Este estudo descreve o desenvolvimento da optimização de um método de HPLC de fase reversa, baseado na norma EN 12856, para a determinação de aditivos alimentares.
A optimização envolveu essencialmente a escolha da fase estacionária e da composição e fluxo da fase móvel, de modo a permitir uma boa resolução cromatográfica dos aditivos alimentares em estudo e simultaneamente diminuir o tempo de análise.
Para além, dos aditivos sacarina, acessulfame K e aspartame, usados como adoçantes, do ácido sórbico e do ácido benzóico, utilizados como conservantes, foram também estudados a cafeína e a teobromina.
Estabelecidas as condições analíticas foram validadas curvas de calibração para as substâncias mencionadas. Foi verificada a existência de linearidade e homogeneidade para a gama de trabalho e foram calculados os limites de quantificação e detecção para cada um dos compostos estudados.

SYNTHESIS OF SINGLE BRIDGED DOUBLE CALIX[4]ARENES

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

Departamento de Engenharia Química, ISEL, Lisboa, Portugal

Calixarenes are well known in supramolecular chemistry for their ability to form host-guest complexes with ionic and neutral molecular species. The synthesis of double (and triple) calixarenes has been attempted by several groups on the expectation that the two (three) binding sites of each calixarene unit could act in cooperativity thus enhancing the molecular/ionic recognition capabilities of all the entity. The connection between the calixarene units have been done through their narrow and wide rims.

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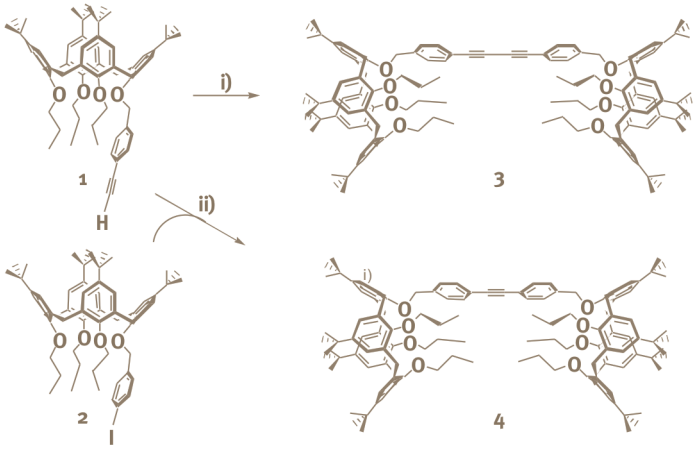

Scheme. Synthesis of double calix[4]arenes.

For the single bridged double calix[4]arene compounds here presented, luminophore properties are expected, which in turn may allow their use as luminescent molecular devices. **3** could be obtained in very good yield (74%) by the oxidative coupling (Glaser type homocoupling) of **1**, while the Sonogashira cross-coupling reaction between **1** and **2** furnished **4** in 56%. Their structures were established by FT-IR, $^{1}H/^{13}C$ NMR, MS and elemental analysis.

CALIX[4]ARENE-BASED POLYMERS: HOMO AND COPOLYMERIZATION WITH CARBAZOLE DERIVATIVES

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

Departamento de Engenharia Química, ISEL, Lisboa, Portugal

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Research in the area of conjugated polymers has attracted significant interest recently in view of their exciting prospects applications in a range of electronic devices. As part of our ongoing research aiming to produce well-defined calixarene-based conjugated polymers as new materials for use in sensing chemistry, the homo and copolymerization of carbazole derivatives (**3-6**) with calix[4]arene units (**1-2**) was examined.

Appropriate calix[4]arene derivatives were successfully functionalized in the lower rim affording the compounds **1** and **2**. The synthesis of carbazole derivatives (**3-6**) was prepared according to reported methods.

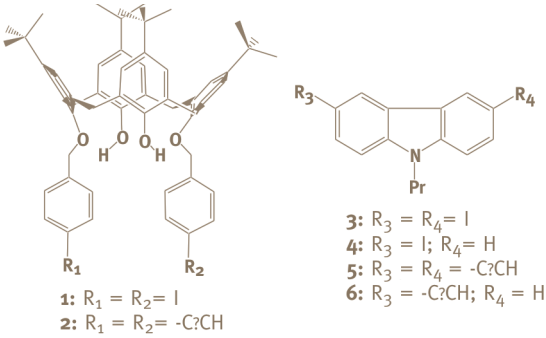

Figure 1. Monomers units

The homopolymerization of **2** and **6** and copolymerization of **1** and **5**, **2** and **3**, **3** and **5** and **2** and **6** were tested under different conditions. The synthesis were accomplished through palladium-catalyzed cross-coupling reactions (7 mol % of $Pd(PPh_3)_2Cl_2$, 7 mol % of CuI and Et_3N in toluene) and Rh(I) as catalyst (2 mol % of $[Rh(nbd)Cl]_2$, 4 eq. Ph_3P in THF) afforded soluble polymers and oligomers with variable conversions. Gel permeation chromatography (GPC) profiles showed multimodal and unimodal distributions. A tentative interpretation of the obtained results will be discussed.

SYNTHESIS AND PROPERTIES OF A NEW POLY(PHENYLETHYNYLENE-CO-DOUBLE CALIX[4]ARENE) FOR MOLECULAR ELECTRONICS

Costa, A.I.[1]; Ferreira, L.F.V.[2]; Prata, J.V.[1]

1 Dept. de Engenharia Química e C. de Investigação de Engenharia Química e Biotecnologia, ISEL, Lisboa, Portugal
2 CQFM-C. de Química-Física Molecular and IN-Institute of Nanoscience and Nanotechnology, IST, Lisboa, Portugal

Publicado em:
Livros de Resumos do 4th International Symposium of Macro and Supramolecular Architectures and Materials – Synthesis, Properties and Applications, Düsseldorf, Alemanha, 7 a 11 de Setembro de 2008.

Conjugated polymers are being used in a broad range of applications such as electrochemical switches, electronic and optoelectronic devices and sensors. Macrocyclic receptors, either as side-chain or main-chain constituents of conjugated polymeric backbones, have been continuously screened as chemical and biological sensors. In comparison to single receptor molecules, conjugated polymer-based sensors show higher sensitivity, leading to higher transduction signal amplification. Only a few studies have so far tackled the potential use of calixarenes as building blocks for this type of supramolecular assemblies. Depending on their specific structural features, these cyclic oligomeric units may act as selective recognition sites for ionic, molecular and biomolecular species thus helping to establish more sensitive interactions of a given analyte with the conjugated polymeric chain, from which the change in their photo/electroluminescence or magnetic properties could provide the necessary transduction element to the sensing device. This work presents the preliminary results on the synthesis and characterization of a conjugated phenylethynylene-type polymer having side-chain *O*-tripropyl-calixarene units, which was primarily designed for sensing chemistry. Poly (phenylethynylene-*co*-double calix[4]arene) (PPE-dCALIX) copolymer here reported (Fig. 1) was prepared by a Sonogashira-type cross-coupling polymerization of a single bridged double calix[4]arene possessing a diiodo functionality (**1**) and 1,4-diethynylbenzene (**2**), with catalytic amounts of $PdCl_2(PPh_3)_2$ and CuI in toluene/NEt_3 at rt (Scheme 1).

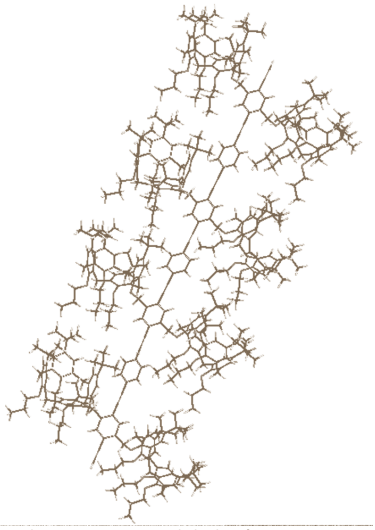

Figure 1. MMFF-minimized structure (tetramer model) of PPE-dCALIX copolymer

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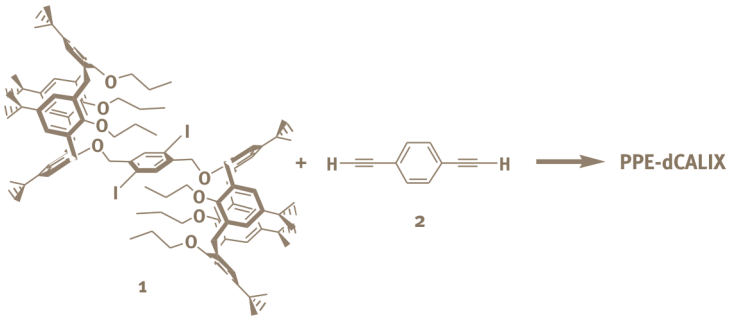
The yellow rod-like copolymer was obtained in almost quantitative yield and the GPC analysis consistently showed a monomodal distribution, with a number-average molecular weight of 23000 $gmol^{-1}$ (M_w/M_n =2.2). Details of its synthesis and characterization will be present.



Scheme 1. Pd/Cu-catalyzed copolymerization of double calix[4]arene (**1**) and 1,4-diethynylbenzene (**2**)

BIOCATALYSIS IN ORGANIC MEDIA BY USING CALIXARENE-MYOGLOBIN COMPLEX WITH PSEUDOACTIVITY OF PEROXIDISE

Semedo, M.C.; Karmali, A.; Barata, P.D.; Prata, J.V.

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

During the last two decades, calixarenes have attracted a great attention both in academic and applied research due to their molecular recognition of biological molecules such as amino acids, proteins and carbohydrates (Ludwig, 2005 and Oshima *et al.*, 2005). Calix[*n*]arenes consist of cup-shaped molecules which can form host-guest complex with a wide range of guest molecules by introducing several functional groups either at the upper or lower rim (Oshima *et al.*, 2005).
The present work involves the use of lower rim substituted acid derivatives of *p-tert*-butylcalix[4,6,8]arene (CAL[4,6,8]-ACID) for selective extraction of myoglobin. All three calixarene compounds were found to extract this haemoprotein to organic phase, exhibiting extraction parameters higher than 0.90. Myoglobin-CAL[6]-ACID complex revealed pseudoactivity of peroxidase which catalysed the oxidation of seryngaldazine in the presence of hydrogen peroxide in organic medium containing chloroform. The effect of pH, protein and substrate concentrations was investigated in biocatalysis by using myoglobin-CAL[6]-ACID complex. The highest specific activity of myoglobin was 1.37 x 10^{-1} U. mg protein^{-1} at initial pH of 6.5 in organic medium. Apparent kinetic parameters ($V'_{máx}$, K'_m, k'_{cat} e k'_{cat}/K'_m) for the pseudoactivity of peroxidase were determined in organic media for different pH values both by Michaelis-Menten and Lineaweaver-Burk plots.
Furthermore, the stability of the protein-calixarene complex was investigated for different initial pH values and $t_{1/2}$ values were obtained in the range of 3.5 – 5.2 days. Myoglobin-calixarene complex present in organic medium was recovered in fresh aqueous solutions at alkaline pH, with a recovery of pseudoactivity of peroxidase over 100% (Semedo, 2008).
The results strongly suggest that the use of calixarene derivatives is an alternative technique for protein extraction and solubilization in organic media for biocatalysis.

Publicado em:
Livro de Resumos do 10th International Chemical and Biological Engineering Conference CHEMPOR 2008, Braga, 4 a 6 de Setembro de 2008.

ONE-STEP PURIFICATION OF HEMOGLOBIN FROM HUMAN ERYTHROCYTES BY USING A NOVEL CHROMATOGRAPHIC MATRIX BASED ON POLYMER-BOUND CALIX[6]ARENES

Semedo, M.C.; Karmali, A.; Barata, P.D.; Prata, J.V.

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

Publicado em:
Livro de Resumos do 10th International Chemical and Biological Engineering Conference CHEMPOR 2008, Braga, 4 a 6 de Setembro de 2008.

Calixarenes are host molecules which exhibit molecular recognition towards a wide range of guest bioactive substances such as amino acids, proteins and carbohydrates (Ludwig, 2005 and Oshima *et al.*, 2002). The complexing abilities shown by these cyclic oligomeric compounds has stimulated their potential use as molecular and biomolecular receptors immobilized on an existing polymeric matrix, for which appropriate grafting methods have been developed (Barata *et al.*, 2004). The present work involves the use of a novel chromatographic matrix based on a polymer-bound acid derivative of *p-tert*-butylcalix[6]arene for one-step isolation of haemoglobin from human erythrocytes. The red cell lysate was applied to a column packed with this matrix which was previously equilibrated in phosphate buffer. The adsorbed proteins were eluted from the column with a linear gradient of Na_2CO_3 pH 11.0 and the column fractions were analysed for protein and pseudoactivity of peroxidase. Human haemoglobin was purified in a one-step procedure with a recovery of pseudoactivity of about 35% and a purification factor of about 12. The purified preparation of haemoglobin was analysed both by SDS and native PAGE which exhibited single proteins bands with Mr of 16.0 and 61.0 KDa, respectively. Furthermore, the single protein band observed in native PAGE was coincident with the pseudoactivity of peroxidase band detected *in situ* on this gel. Protein adsorption on this novel chromatographic matrix involved several interactions such as electrostatic and hydrophobic and other parameters affected this process such as protein size, pI, pH, ionic strength and nature of buffer ion (Semedo, 2008).
The results strongly suggest that this novel chromatographic matrix presents some advantages over other matrices as far as selectivity is concerned for protein purification.

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

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Tomato pomace and pectin were used as the sole carbon sources for production of polygalacturonase from a strain of *Coriolus versicolor* in submerged culture. The culture of *C. versicolor* grown on tomato pomace exhibited a peak of polygalacturonase activity (1427 U/L) on the 3rd day of culture with a specific activity of 14.5U/mg protein. The production of polygalacturonase by *C. versicolor* grown on pectin as sole carbon source, increased with the time of cultivation, reaching a maximum activity of 3207 U/L of fermentation broth with a specific activity of 248 U/mg protein. Differential chromatographic behaviour of lignocellulosic enzymes produced by *C. versicolor* (*i.e* polygalacturonase, xylanase and laccase) was studied on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion were studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The adsorption of polygalacturonase as well as other enzymes to immobilized metal chelates was due to coordination of histidine residues which are available at the protein surface since the presence of imidazole in the equilibration buffer abolished the adsorption of the enzyme to immobilized metal chelates. A one-step purification of polygalacturonase from *C. versicolor* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II) and purified enzyme exhibited a specific activity of about 150 U/mg protein, final recovery of enzyme activity of 100% and a purification factor of about 10. The use of short spacer arm and the presence of imidazole in equilibration buffer exhibited a higher selectivity for purification of polygalacturonase on this column with a high purification factor. The purified enzyme preparation was analysed by SDS-PAGE as well as by "*in situ*" detection of enzyme activity.

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DEVELOPMENT OF A BIOSENSOR BASED ON ION-SELECTIVE ELECTRODE FOR UREA IN MILK BY USING IMMOBILIZED AMIDASE FROM *Pseudomonas aeruginosa*

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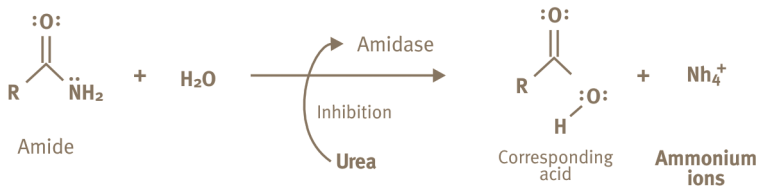
The food processing industry requires suitable analytical methods for quality control of food which are fast, reliable, specific and cost-effective since current wet chemistry tests are time-consuming and some may require highly skilled labour as well as expensive equipment (Verma *et al.*, 2003). This urgent need is due to increased regulatory action and consumer concern about food composition and safety (Luong *et al.*, 1997).

Milk has been considered as a human's most nearly perfect food as far as nutritional properties are concerned and its consumption depends on strict sanitary control employed by the dairy industry (Potter and Hotchkiss, 1995). Urea is present as an adulterant in milk since it is not a natural constituent of milk which has originated increasing concern from the public as the consumer. The presence of urea in milk may be due to excessive nitrogen uptake whose concentration is in the range of 1.66 – 4.16 mM and high urea concentrations are responsible for reduced fertility rates in dairy cattle (Butler *et al.*, 1996)

The present work involves the development of a biosensor based on ion-selective electrode (ISE) for assay of urea in milk by using a novel enzymatic method. Urea is a powerful time-dependent active-site directed inhibitor for aliphatic amidase (acylamide amidohydrolase EC 3.5.1.4) from *Pseudomonas aeruginosa* which catalyses the hydrolysis of a small number of aliphatic amides producing the corresponding acid and ammonia (Martins *et al.* 2006; Tata *et al.*, 1993) according to the following reaction:



Increasing concentrations of urea were found to inhibit proportionally amidase activity which was detected by the hydrolase reaction. Therefore, urea concentration in samples was inversely proportional to amidase activity which was measured with acetamide as substrate by using ISE for ammonium ions.
Cell-free extracts containing amidase activity were immobilized on nylon and polyethersulfone membranes in the presence of gelatin and glutaraldheyde as the bi-functional reagent. Membranes containing immobilized amidase activity were used to set up a biosensor based on ISE for ammonium ions by using acetamide as the substrate and the enzyme reaction was followed by measurement of ammonium ions due to hydrolysis of the aliphatic amide (Fig.1).

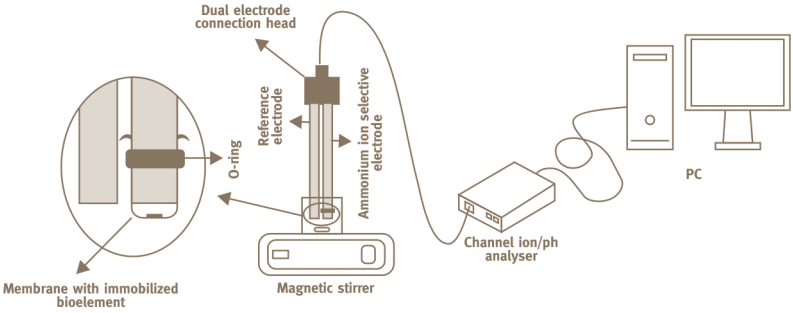


Figure 1. Experimental set-up for potentiometric biosensor: ammonium ion selective electrode containing polyethersulfone membrane with immobilized enzyme and reference electrode, electrochemical cell, magnetic stirrer, ISE analyser and PC.

Subsequently, this biosensor was washed and incubated with milk containing increasing concentrations of urea in the range of 0 - 11µM, for 1h. After the incubation period, the biosensor containing amidase activity was assayed again by using acetamide as the substrate. There was a linear relationship between a decrease of the biosensor response in mV and urea concentration in milk. This biosensor exhibited a linear response in the range of 2.0 – 10.0 x 10^{-6} M of urea either in a buffer solution or in milk and a response time of 60s. The biosensor containing amidase activity could be re-used again by reactivating enzyme activity with hydroxylamine for 2h. This biosensor was stable for at least 1 month since it did not lose enzyme activity and it is cheap because cell-free extracts containing amidase activity can be used for quantification of urea in milk.

PRODUCTION AND CHROMATOGRAPHIC BEHAVIOUR OF POLYGALACTURONASE FROM Pleurotus ostreatus ON IMMOBILIZED METAL CHELATES

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A strain of *Pleurotus ostreatus* was grown in submerged culture in tomato pomace as sole carbon source for production of polygalacturonase. The culture of *P. ostreatus* revealed a peak of polygalacturonase activity (2181 U/L) on 4th day with specific activity of 42.8 U/mg protein. Differential chromatographic behaviour of polygalacturonase, xylanase and laccase from *P. ostreatus* was investigated on immobilized metal chelates. The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion was studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The presence of imidazole in the equilibration buffer abolished the adsorption of the enzymes to immobilized metal chelates. A one-step purification of polygalacturonase from *P. ostreatus* was devised by using a column of Sepharose 6B-EPI 30-IDA-Cu(II). Purified enzyme exhibited a specific activity of about 1600 U/mg protein, final recovery of enzyme activity of 80% and a purification factor of about 65. The purified enzyme preparation was analysed by SDS-PAGE as well as by *in situ* detection of enzyme activity. Purified preparation of polygalacturonase exhibited a pH and temperature optima of activity at 7.0 and at 50°C, respectively. The kinetic parameters (V_{max}, K_m, K_{cat}, and K_{cat}/K_m) of purified enzyme were found to be 5530.8 ± 260.7 U/mg of protein, 13.23 ± 2.79 mg/ml of polygalacturonic acid, 5553.01 ± 261.7 s^{-1} and 419.72 $s^{-1}.mg^{-1}$, respectively. Purified enzyme exhibited a half life (t 1/2) of 60 ± 7.45 min and 35 ± 0.37 min at 50°C and at pH 6.0 and 7.0, respectively.

PRODUCTION, PURIFICATION AND PARTIAL CHARACTERIZATION OF PROTEIN – BOUND POLYSACCHARIDES FROM *Pleurotus ostreatus* AND *Lentinula edodes*

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The medicinal power and the nutritional value of some mushrooms are widely known. However, only in the last decades of the last century that it was possible to isolate and partially characterize some biologically active anti-cancer substances [Chaplin *et al.*, 1994].

The therapeutic properties of mushrooms are attributed mainly to their polysaccharide content which has exhibited immunomodulatory properties such as anti-cancer, anti-viral and anti-bacterial activities. Protein-bound polysaccharides are macromolecules which consist of a central core protein to which are attached a number of polysaccharide chains and PSP and PSK from *Coriolus versicolor* are the most widely studied protein-bound polysaccharides. [Parris *et al.*, 2000; Cui & Chisti, 2003]

Although protein–bound polysaccharides from mushrooms exhibit important medicinal properties, there is little information in the literature about their biological and physico-chemical properties. [Cui & Chisti, 2003; Huie & Di, 2004; Lo *et el.*, 2007]

Therefore, the aim of this work consists of production, purification and partial characterization of these protein-bound polysaccharides from *Pleurotus ostreatus* and *Lentinula edodes*.

The fungal strains were grown in several culture media such as whey permeate supplemented with glucose, yeast extract and suitable salts. The cultures were grown in agitated and aerated bioreactors at pH 5.5 and 27ºC, with pH and temperature control for 10 days and suitable daily samples were removed from the reactor. These samples were centrifuged and intracellular and extracellular protein-bound polysaccharides were extracted from the biomass and culture supernatant, respectively. Subsequently, these polysaccharides were purified by gel filtration chromatography on a Sephacryl HR-100 column and fractions were analysed for protein, superoxide dismutase (SOD) activity and polysaccharides. Fractions containing protein-bound polysaccharides were characterized by HPLC which revealed UV and RI peaks with retention times of 6 and 13 min., respectively. On the other hand, FTIR analysis of these polysaccharide preparations revealed absorption peaks at 912, 1083, 1458, 1653, 2943 and 3409 cm^{-1} which are charac-

teristics of such macromolecules. Moreover, purified polysaccharides exhibited SOD activity which is in agreement with the data published in the literature. [Cui *et al.*, 2007; Wang *et al.*, 2007, Peng *et al.*, 2003; Kim *et al.*, 2003].

The results presented strongly suggest that these basidiomycete strains produce high levels of free and protein-bound polysaccharides which exhibit similar physico-chemical properties compared with the data in the literature as far as HPLC and FTIR analysis are concerned.

OVERPRODUCTION OF PROTEIN-BOUND POLYSACCHARIDES FROM A Coriolus versicolor STRAIN BY SUBMERGED FERMENTATION

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Several species of mushrooms have been valued as edible and medicinal resources. Polysaccharides mushroom-derived have shown medicinal effects such as blood pressure and cholesterol lowering, liver protection, anti-fibrotic, anti-inflammatory, anti-diabetic and anti-viral activities. Additionally, some strains are able to synthesize new polysaccharopeptides with antitumoral and immunostimulating properties (Cui *et al.*, 2007; Li *et al.*, 2008). The protein-bound polysaccharides or polysaccharopeptides, produced by the white rot fungus, *Coriolus versicolor*, are effective immunopotentiators used to supplement the chemotherapy and radiotherapy of cancers and various infectious diseases (Cui and Chisti, 2003).

The aim of this study was to define experimental conditions to optimize the production of protein-bound polysaccharides by *C. versicolor*. Most of the reported studies referred polysaccharides isolated from mycelium, however a few studies on exopolysaccharides from *C. versicolor* have been reported (Kim *et al.* 2002; Tavares *et al.* 2005). In fact, the polysaccharides represent the major constituent that establishes the rigidity and morphological properties of the fungal cell wall and, depending on the culture conditions, they can be excreted to the medium. In this work, endo and exoprotein-bound polysaccharides, produced by *C. versicolor* will be investigated. In order to evaluate and to optimize the production of these compounds we performed submerse cultures with four different carbon sources: glucose, maltose, sucrose and manitol. Additionally, aiming for a clean process and to reduce the medium cost, two kinds of agro-industrial residues were used: tomato pomace and beet wastes.

C. versicolor was isolated from *Quercus suber* L. and kindly provided by ISEL. The culture was maintained on PDA, transferred to a fresh agar plate every month, and grown at 28 ºC for approximately 7 days. The mycelia of *C. versicolor* on the media surface were cut and transferred to culture flasks. The cultures were prepared in shake-flask with a basal media comprised by the following ingredients per liter: yeast extract 2 g, KH_2PO_4 0.8 g, $MgSO_4.7H_2O$ 0.5 g, $Na_2HPO_4.2H_2O$ 0.25 g, NH_4NO_3 1 g, pH 6.0. The different carbon sources were added one by

one to the basal medium. Flasks were incubated at 28ºC, for 20 days using an orbital shaker at 150 rpm. Samples were collected periodically along the twenty days of the assays. The exopolysaccharides were extracted from the supernatant according to Lin and Sung (2006) and the polysaccharide concentration was determined by the phenol–sulphuric method (Dubois *et al.*, 1956). Protein-bound polysaccharide concentration obtained in the batch cultures ranged between 150-900 $\mu g.mL^{-1}$. The highest polysaccharide concentration was achieved with tomato pomace as agro-industrial residues corresponding to the 14th day of culture. Based on these results *C. versicolor* was cultivated in the basal medium plus tomato pomace in a stirred bioreactor during 15 days, for the production of endocellular and exocellular protein-bound polysaccharides. The intracellular polysaccharides extraction was performed from the mycelia according to Lee *et al.* (2006) and Gern *et al.* (2008). Endocellular and exocellular protein-bound polysaccharides were quantified as described previously. The concentration of the polysaccharide compounds was 16 folds higher in the supernatant, than in mycelia. Absorption spectra of both polysaccharides have a maximum at 280 nm, however, supernatant complex has a protein concentration 40 folds higher than mycelia, showing the production of different protein-bound polysaccharides by this strain.

The comparison of the results obtained in this study with those reported in the literature, let us to confirm the interest of this selected culture medium in order to maximise the production of complexes protein-polysaccharides by *C. versicolor*. Besides, this clean process allows valuing the agro-industrial residues with a low cost and a higher production of these polysaccharides compounds. The different polysaccharide concentration in endocellular and exocellular complexes shows that this *C. versicolor* strain produces different protein-bound polysaccharides, so further studies are being done in order to isolate and identify the different *C. versicolor* complexes and investigate its bioactivity.

STRUCTURAL AND KINETICS EFFECTS OF *Pseudomonas aeruginosa* WILD-TYPE AMIDASE ENCAPSULATION IN REVERSED MICELLES

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Publicado em:
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Amidases(E.C. 3.5.1.4) which in nature catalyze the hydrolysis of amide bonds in small aliphatic amides has also the capacity to catalyse the acyl group transfer to amines, such reaction enlarges the possibility of synthesizing different compounds containing amide bonds (Pacheco *et al.*, 2005).
The reaction catalysed by amidase involves a ping-pong bi-bi mechanism with the formation of an acyl-enzyme complex that is able to transfer the acyl group either to an amine or to the water present in the system, with formation of the transamidation or the hydrolytic product, respectively.

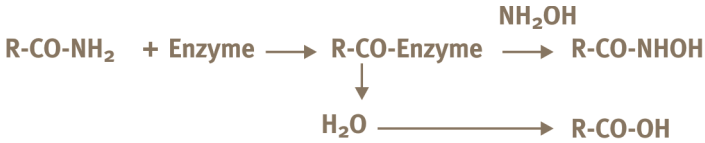

Figure 1. Aliphatic amidase catalyses the hydrolysis and transamidation reactions of amides.

Hydroxamic acids derivatives, with the general formula R–CO–NHOH, are products of the former transamidation reaction when the acyl acceptor is hydroxylamine. Hydroxamic acids are chelating agents which are known to inhibit metalloproteinases often associated to several human pathologies. These compounds might be used in a number of interesting applications, such as in medicine and neurobiochemistry in several drugs since they are constituents of grow factors, antibiotics, antibiotic antagonists, tumor inhibitors and antifungal agents. On the other hand, hydroxamic acids can also be applied in food industry and waste-water treatment (Fournand *et al.*, 1997a). Regarding the above reaction scheme, such transamidation reaction can be successfully performed in an organic media since the water content is low (Fournaud *et al.*, 1997). Reversed micellar systems are one such example of the use of nonconventional media for hydroxamic

acid synthesis using amidase (Pacheco *et al.*, 2005).
Reverse micelles are spherical waterdroplets surrounded by a monolayer of closely packed surfactant molecules dispersed in a solvent of low polarity. In reverse micelles, the polar heads of the surfactant molecules are in contact and hydrated by few water molecules that lie in the interior of the micelle; the hydrophobic tails of the surfactant molecules are oriented and in contact with the surrounding organic solvent (Gómez –Puyou and Gómez –Puyou, 2007).
The present work involves the entrapment of either purified recombinant amidase, cell-free extract or whole cells from *Pseudomonas aeruginosa* (E.C.3.5.1.4) in a reversed micellar system composed of cationic surfactant tetradecyltrimethyl ammonium bromide (TTAB) in heptane/octanol (80/20% V/V). Our work reports the effect of the enzyme entrapment in both catalytic activity of acetohydroxamic acid synthesis and amidase structure. The results obtained revealed that there was an increase in enzyme activity for the synthesis of acetohydroxamic acid in reverse micelles compared with the conventional aqueous system.
Reverse micelles are optically transparent. When enzymes are transferred to the interior of reverse micelles, the system continues to be transparent, and, thus the entrapped enzyme is susceptible to spectroscopic studies (Gómez –Puyou and Gómez –Puyou, 2007). Fourier Transform Infrared Spectroscopy (FTIR) was used to analyze structural differences on amidase by using medium engineering since in a wide range of environments (Haris and Severcan, 1999).
FTIR analysis revealed modifications on secondary structure of encapsulated amidase since amidase structure exhibited mainly α-helices (1650-1655 cm^{-1}) as opposed to the enzyme structure in aqueous solution witch shows as predominant β-sheet (1620-1620 cm^{-1}). The results obtained from FTIR spectra in conjunction with biocatalysis of amidase strongly suggests that the synthesis of acetohydroxamic acids is higher with α-helical structure compared with β-structure. Our findings clearly demonstrated some advantages in the use of encapsulated amidase in reverse micelles for synthesis of acetohydroxamic acids compared with aqueous system as well the importance of structural modification on amidase molecule for high yield of transamidation products.

ANALYSIS OF PRODUCTION OF RECOMBINANT WILD-TYPE AMIDASE FROM Pseudomonas aeruginosa IN Escherichia coli

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High level of expression of recombinant proteins often results in aggregation and accumulation in inclusion bodies hindering the production of large amounts of protein. *Escherichia coli* retains its dominant position as the first choice of host for reasons of speed and simplicity (Middelberg, 2002). However there is a disadvantage when protein are overexpressed, that is the formation of inclusion bodies. Inclusion bodies are dense aggregates of misfolded polypeptide and they are formed intracellularly because of the aggregation characteristics of the protein or the inability of the cellular processes to ensure that the expressed protein is soluble and correctly folded (Lilie *et al.*, 1998). This may facilitate their potential purification because inclusion bodies are usually highly homogeneous. The problem is that renaturation is frequently difficult, as a result of aggregation. The latter applies to those proteins for which renaturation is a problem with expensive high-through put operations of *in vitro* refolding following chemical denaturation (Thomas and Baneyx, 1997). Here the only way out is to avoid or at least reduce the inclusion body formation. Thus, it is desirable to produce recombinant proteins in a soluble conformation in vivo and to purify the active polypeptide by traditional chromato-graphy techniques.

The reduction of the cultivation temperature is known to increase the amount of native protein due to the decrease in the rate of the protein synthesis. The increase native protein is limited by the induction of gene expression by the promotors, which can be linearly regulated by the inducer concentration. This strong correlation between cultivation temperature and inducer concentration, IPTG, with the expression level and the solubility of the recombinant protein has also been found in several studies (Garcia-Junceda *et al.*, 1995).

Protein folding *in vivo* is mediated by helper proteins termed molecular chaperones (Nam and Walsh, 2002). When *E.coli* is subjected to a variety of stresses the synthesis of 20-30 heat-shock proteins is transiently increased in order to repair cellular damage. The heat shock response controls the levels of chaperones and proteases in order to ensure a proper cellular environment for protein folding

(Guisbert et al, 2004). Ethanol is one of the most powerful elicitors of the heat shock response in *E.coli*, several studies show that alcohol shock with ethanol can induce the synthesis of intracellular chaperones (Nam and Walsh, 2002).
Thomas and Baneyx (1997) have reported that supplementing the grown medium with 3% ethanol can be a powerful tool to improve the solubility of certain recombinant proteins. But this effect could not be fully explained by higher intracellular concentration of molecular chaperones since there is always a lower protein synthesis rate in ethanol treated cultures (Thomas and Baneyx, 1997). It is clear that a slow expression of the desired protein will facilitate the correct folding of the protein which will promote an increase in the solubility of the recombinant protein.
Microbial amidases, which in nature catalyse hydrolysis of an amide compound to a carboxylic acid and ammonium, have been used for applications in diverse fields such as neurobiochemistry (Cravatt *et al.*, 1996), plant physiology, medicine, environment and in the food and detergent industry (Fournaud *et al.*, 1998). In this study, the combination of parameters such as temperature incubation, IPTG induction and 3% ethanol supplementation of LB ampicilin culture medium in the prevention of the *in vivo* aggregation of this protein with the aim to improve the expression level of active recombinant protein and to minimize the formation of inclusion bodies by *Escherichia coli* overproducing *Pseudomonas aeruginosa* native amidase (E.C. 3.5.1.4).

MEASUREMENT AND CORRELATION OF SOLUBILITY OF RED 153 IN SUPERCRITICAL CARBON DIOXIDE

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Solubility measurements of red 153 in supercritical carbon dioxide were carried out in a flow type apparatus, at the temperature range from 323 to 393 K and for pressures from 15 to 40 MPa. The dynamic apparatus consists of the usual three sections of compression, equilibrium and expansion but some modifications have been introduced. The supercritical fluid mixture including the dye was released at the expansion valve and the dye was trapped in a system of filters without organic solvents. The dye precipitated in the system during the depressurization was recovered by washing out with methanol and analyzed in a UV-Vis spectrophotometer. The values of solubility change from 9.35×10^{-7} to 3.71×10^{-5}. Semi empirical density-based models were used to correlate the solubility of red 153 in supercritical carbon dioxide. From the correlation results, the head of red 153-CO_2 solvation and that of solute dye vaporization were determined and compared with the results in literature.

Publicado em:
Proceedings of the 11th European Meeting on Supercritical Fluids, Barcelona, (Spain), 4-7 Maio de 2008, pp. 1-4.

VOLUMETRIC PROPERTIES FOR THE TERNARY MIXTURE METHANOL-FOR MAMIDE-ACETONITRILE

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Densities have been measured for the ternary mixture methanol-formamide-acetonitrile as a function of mole fraction at 298.15 K. The correspondent molar volume was determined along with two relevant connected properties: the excess molar volume and the partial molar volume of the mixtures. Excess molar volumes of the binary mixtures have been fitted with a Redlich-Kister type relationship and ternary fractions with the Cibulka polynomial relationship. Results have been used to interpret the nature of solvent-solvent interactions among mixtures' components.

TOWARDS THE TESTING OF AN ALTERNATIVE METHOD FOR MULTICRITERIA ANALYSIS OF CUSTOMER SATISFACTION

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This paper presents a method for customer satisfaction analysis in which the aggregation of the individual customer satisfaction criteria into an overall value function uses dummy variable regression technique with additional constraints and employs the least squares approach. The value for each level of the value functions is calculated by means of the coefficients of the dummy variables. For finding the coefficients several different forms of implementation have been used namely differences to a reference level considering several different reference levels. The quality of the results produced by the method was tested with real survey data from the hospitality industry. The results obtained with the new method for measuring and analyzing customer satisfaction were also compared with MUSA methodology based on the aggregation of individual judgments into a collective value function via a linear programming disaggregation formulation. The major findings from this analysis will be discussed in this paper.

Publicado em:
Proceedings do 19th International Conference on Multiple Criteria Decision Making, MCDM 2008, Auckland, New Zealand, 7 a 12 de Janeiro de 2008, pp. 134.

KEY QUALITY DIMENSIONS FROM THE CUSTOMER'S POINT OF VIEW: A CASE STUDY IN TWO PORTUGUESE HOTELS

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Publicado em:
Proceedings do IEMC - Europe 2008, International Engineering Management Conference, Managing Engineering, Technology and Innovation for Growth, Estoril, 28 a 30 de Junho de 2008, IEEE International, pp. 88-91.

This paper analyses the strengths and weaknesses of critical incident technique (CIT) when applied as a tool to identify the key quality dimensions to be used as criteria to generate and evaluate intervention strategies. Using CIT, a total of 679 incidents were gathered from two Portuguese hotels, regarding satisfying or dissatisfying episodes with the provided service. The incidents were categorized and the service quality dimensions identified. The scores reflecting the extent to which the quality dimensions are achieved are useful to establish and prioritize improvement actions.

ANÁLISE DA SATISFAÇÃO DE CLIENTES NA INDÚSTRIA HOTELEIRA: APLICAÇÃO DE METODOLOGIAS MULTICRITÉRIO DE APOIO À DECISÃO

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A satisfação do cliente tornou-se nas últimas décadas um assunto de grande relevância para organizações das mais variadas dimensões e áreas de negócio. A satisfação do cliente é um objectivo operacional chave para muitas organizações. As empresas congregam esforços para aumentar o seu desempenho em áreas que têm grande contribuição para a satisfação do cliente. No entanto, muitas organizações não sabem qual o resultado dos seus esforços pois em geral não medem a satisfação dos seus clientes, ou fazem-no de forma inadequada. Este trabalho tem como objectivo analisar a satisfação do cliente usando para tal dois métodos distintos. O primeiro baseia-se no uso dos conjuntos aproximativos e representa as preferências dos clientes através de regras de decisão simples do tipo "se o atributo x é considerado bom e o atributo y é considerado suficiente então a avaliação global do produto é média". A capacidade de representar as preferências dos clientes em expressões do tipo "se"..."então", torna esta metodologia interessante do ponto de vista da gestão. O segundo método usado baseia-se na construção de funções de valor as quais têm um papel de relevo nos modelos de preferência usados na análise multicritério de apoio à decisão. O método a usar consiste num modelo de desagregação de preferências o qual segue os princípios da análise de regressão ordinal. Recorrendo a um conjunto de dados provenientes da indústria hoteleira apresentam-se os resultados obtidos com os dois métodos usados e retiram-se conclusões sobre a sua utilização na análise da satisfação do cliente.

Publicado em:
Actas do 13º Congresso da Associação Portuguesa de Investigação Operacional, IO 2008, Vila Real, 17 a 19 de Março de 2008, pp. 47.

04

PERFORMANCE INDICATORS FOR REACTIVE DISTILLATION DESIGN

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A cost indicator for the design and multi-objective optimization of reactive distillation columns, designated capacity, was introduced in previous work by the authors. The question of this indicator's effectiveness as a measure of the actual column cost, is herein investigated over a number of designs by comparing it with the value obtained by means of conventional costing procedures. The results show that the level of accuracy obtained when using capacity is satisfactory and certainly acceptable for a preliminary design stage.

ADAPTIVE FEEDBACK LINEARIZING CONTROL FOR TRANSPORT PHENOMENA PROCESSES

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Adaptive feedback linearizing control of distributed plants involving transport phenomena, described by partial differential equations is considered. The method proposed relies on Lyapunov's stability to obtain parameter estimates and tackles directly infinite dimension systems without finite dimension approximations. The control of a tubular countercurrent heat exchanger is presented as an example to illustrate the method.

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Proceedings do CONTROLO 2008, 8th Portuguese Conference on Automatic Control, 21 a 23 de Julho de 2008, UTAD, Vila Real, Portugal.

COMBUSTÃO CATALÍTICA DO TOLUENO SOBRE CuZSM-5 SUPORTADO EM ESPUMAS CERÂMICAS

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Catalisadores zeolíticos do tipo CuZSM-5 suportados em espumas cerâmicas de cordierite foram utilizados na reacção de oxidação total do tolueno. A camada de revestimento do zeólito na espuma mostrou-se muito uniforme com uma espessura média de 27 ± 1 µm e com uma boa aderência à superfície da espuma de cordierite (perdas da ordem de 0,4% em massa). A espuma revestida com 4,5% em massa de CuZSM-5 revelou bom comportamento catalítico na oxidação total do tolueno. Com efeito, quando se utiliza o catalisador na forma de pó é necessário utilizar uma quantidade cerca de 3 vezes superior para obter os mesmos resultados catalíticos. Por outro lado, quando se comparam resultados com massa equivalente de fase activa verifica-se uma redução da temperatura de "light-off" de 30ºC.

CATALYTIC COMBUSTION OF VOCS OVER METAL ZEOLITES SUPPORTED ON CORDIERITE FOAMS

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As catalysts supports, open-cell ceramic structures (reticular foams) are preferred, since they can provide lower pressure drops as well as good mixing of the reactants, leading to potential improvements on the catalytic efficiency. Several processes have been developed to produce these foams, being the replication method the most widely spread. However, one of the major drawbacks of this replication process is the presence of triangular hollow cavities in the struts of the structure, also possessing sharp corners due to the burnout of the polymeric sponge. Hence, there is a need to develop improved processing methods. In this work a new developed process, named direct foaming, is proposed to produce reticulated cordierite foams. Replicated cordierite foams were coated with platinum and copper-based zeolite catalysts by a washcoating method, being after evaluated for the isopropanol and toluene total combustion.

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Proceedings of the Conference du Groupement De Recherche International, Catalysis for Environment: Depollution, Renewable Energy and Clean Fuels, Zakopane, Poland, September 2008, pp. 201-206.

NONLINEAR DYNAMIC MODELING OF A REAL PILOT SCALE CONTINUOUS DISTILLATION COLUMN FOR FAULT TOLERANT CONTROL PURPOSES

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The aim of the present work is to develop and validate a nonlinear dynamic model of a pilot-scale continuous distillation process for the simulation of the dynamic behaviour of a real continuous distillation plant at the Chemical Engineering Department of ISEL, in the absence and in the presence of faults. The model of the overall pilot scale distillation plant is derived from fundamental principles including mass and energy balances for the individual systems such as the distillation column sections, the condenser, the heated reboiler, the feed pre-heater, the reflux valve, the bottom product control valve and the PID regulatory level controller. The complete dynamic model for the separation of a non-ideal binary liquid mixture of ethanol/water was developed within Matlab®/Simulink environment and was validated against experimental data collected from the plant under normal operating conditions in the absence and in the presence of faults showing a good agreement with the experimental results. Thus, this non-linear dynamic model is well-suited to be used for the implementation of Fault-Tolerant Control strategies in real time.

BIFUNCTIONAL CATALYSTS BASED ON MCM-22 ZEOLITE. THE ROLE OF Pt INTRODUCTION METHOD

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The behaviour of bifunctional catalysts based on MCM-22 zeolite was investigated in transformation of n-hexane. The Pt was introduced by ion exchange, incipient wetness impregnation and mechanical mixture with Pt/Al2O3. The method used affects the location of metal particles at the internal/external surface of MCM-22 zeolite and, consequently, influences the location of catalytic reactions. In n-hexane transformation the strong deactivation observed in the first minutes of reaction is attributed to the occurrence of the reaction inside the supercages. After the initial deactivations the reactions proceed at the external surface (both impregnated and ion exchanged catalysts) and inside the sinusoidal channels (ion exchanged sample).

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PREPARAÇÃO DE CARVÕES MESOPOROSOS USANDO COMO MATRIZ ARGILAS POROSAS HETEROESTRUTURADAS

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Livros de Resumos da XXXIII Reunión Ibérica de Adsorción, Madrid, Espanha, 22 a 23 Setembro de 2008.

Desde o trabalho de R. Ryoo el al. que em 1999 apresentou a síntese do primeiro carvão mesoporoso com estrutura regular (amostra designada por CMK-1), que o estudo deste tipo de materiais tem despertado grande interesse na comunidade científica, pelas potencialidades deste tipo de carvões para um largo número de aplicações em áreas emergentes, como o armazenamento de energia, a adsorção ou mesmo a catálise heterogénea, actuando como suportes de catalisadores. A estratégia de síntese dos carvões mesoporosos regulares tem como base a utilização de uma material inorgânico mesoestruturado. Os principais passos do processo de síntese são: i) síntese da matriz inorgânica; ii) infiltração do precursor de carbono (geralmente um polímero ou pré-polímero) na estrutura porosa da matriz; iii) polimerização do percursor de carbono; iv) carbonização do compósito formado anteriormente e v) remoção da matriz inorgânica, usualmente por ataque com HF. A estrutura e textura dos carvões está dependente de vários parâmetros experimentais, sendo, obviamente, o tipo de matriz inorgânica um dos mais determinantes. Assim, para além de sílicas das famílias MCM e SBA, empregues nos primeiros estudos, têm igualmente sido usados outros tipos de materiais inorgânicos como matrizes. A título de exemplo podem referir-se os estudos onde se usaram zeólitos e o estudo onde, recentemente, D. Nguyen-Thanh e T.J. Bandosz mostrarm que também as argilas porosas heteroestruturadas – do inglês Porous Clay Heterostructured (PCH) – podem ser usadas como matrizes para a síntese de carvões mesoporosos. Na presente comunicação apresentam-se os resultados do estudo que teve como objectivo avaliar de que modo o método de preparação das PCHs (concretamente o tipo de amina usada na intercalação) vai influenciar a estrutura do carvão preparado tomando-as como matriz.

PROTOCOLOS EXPERIMENTAIS YOUTUBE

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São cada vez mais complexos e sofisticados os procedimentos e equipamentos usados no ensino das técnicas experimentais em química. O número de alunos em cada aula tem vindo também a aumentar. Os professores são ainda confrontados com o desafio de ensinar diferentes técnicas à mesma turma em escassas horas. Quanto aos alunos, têm não só de aprender a técnica proposta, bem como o funcionamento dos equipamentos envolvidos num tempo reduzido.
A subjugação do processo de aprendizagem de uma nova técnica às dificuldades de operação do equipamento afasta os alunos do essencial: a compreensão científica do método que estão a aprender.
De modo a ultrapassar as dificuldades enunciadas criou-se um ambiente virtual que simula a experiência que os alunos vão encontrar no laboratório. São disponibilizadas via www folhas de hipertexto desenvolvidas contendo elementos multimédia como filmes e fotos, blocos interactivos baseados em flash ou javascript. Os alunos podem assim ensaiar o protocolo experimental antes de o realizar, focando a sua atenção nos aspectos conceptuais. Os alunos encontram um laboratório virtual idêntico ao que irão encontrar na realidade. Cada equipamento é apresentado através de um filme em que se explica o seu funcionamento. Quando os alunos chegam ao laboratório para realizar os ensaios já se encontram familiarizados com as funções e comandos mais importantes do equipamento e também com os principais passos da experimentação.
Esta abordagem envolvendo tecnologias de informação baseadas na internet tem-se revelado bastante positiva. Os alunos mostram-se mais confiantes e autónomos nos procedimentos operacionais e centrados no problema científico em estudo. Utilizam-se técnicas de comunicação permitidas pelos actuais meios informáticos e que nos permitem inovar para além dos protocolos em papel.

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Livro de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, 11 a 13 de Junho de 2008, FEUP, Porto, pp. 287.

AVALIAÇÃO DA SATISFAÇÃO DO CLIENTE NO SECTOR DO TURISMO EM PORTUGAL

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Ciclo de seminários do CEG-IST, IST Taguspark, 6 de Outubro de 2008.

De modo que o sector do turismo nacional se possa desenvolver e consolidar no futuro, este tem de ser pautado por intervenções de desenvolvimento que se fundamentem em estudos técnico-científicos rigorosos. A satisfação do cliente não surge como uma opção mas como uma questão fulcral para o êxito do sector, pois este depende em grande medida do agrado, retenção e fidelidade dos seus clientes. Nesta comunicação faz-se uma análise critica aos principais tipos de métodos usados na avaliação da satisfação do cliente no sector do turismo e apresenta-se o trabalho decorrente do desenvolvimento e teste de um método para avaliação da satisfação do cliente no sector do alojamento turístico.

A DUMMY VARIABLE REGRESSION METHOD FOR CUSTOMER SATISFACTION ANALYSIS

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One of the main tasks in customer satisfaction analysis is the correct handling of the information provided by the customers. The data are usually obtained via questionnaires and directly from the customers' judgments which have a qualitative rather than a quantitative nature. A new method for measuring and analyzing customer satisfaction is presented. To estimate the basic model it is used a dummy variable regression with constraints. The method can very simply make use of qualitative data by codification of the criteria levels being possible to exploit the qualitative judgments of the customer. The mathematical model expresses the fundamental relationship between criteria and the overall value which expresses the global customer satisfaction.

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CATALYTIC COMBUSTION OF TOLUENE ON CU AND PT MFI ZEOLITES SUPPORTED ON CORDIERITE FOAMS

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Background

The emission of volatile organic compounds (VOCs) to the atmosphere is an important environmental problem. Catalytic oxidation is one of the most suitable ways for VOCs removal from numerous gas effluents. Recently, ceramic foam catalyst supports have revealed potential improvements on the catalytic efficiency. In this work cordierite foams, produced by replication method, have been washcoated with Cu and PtMFI zeolites. The catalytic properties of zeolite based foams were evaluated in the deep oxidation of toluene.

Results

Cu and Pt MFI zeolites supported on cordierite foams prepared by an improved washcoating method, involving a cationic polymer and powder metal zeolite suspensions, revealed uniform catalyst layers, with thicknesses in a range of 25-50 m for catalyst contents between 5-20 wt.%. Negligible weight losses, after 1h ultrasounds, show good adhe-rence of the coatings onto the foam's surface. CuMFI (2 wt.% Cu) and PtMFI (0.1 wt.% Pt) coated cordierite foams, with catalyst contents around 5-8 wt.%, have been evaluated in the toluene total oxidation (800 ppm in air). They show higher catalytic activity than their bulk-form counterparts. High oxidation rates and a decrease of about 50°C in the light-off temperature (temperature at which 50% of toluene conversion into CO_2 is attained) were obtained with foam based catalysts. Bulk-form catalysts require the use of higher catalyst contents (about 2 - 3 times more) to obtain similar toluene conversions. Besides the activity increase, for Cu based foams, the dispersion of metal zeolites into thin coatings also provides higher selectivities into CO_2 (negligible CO formation). The enhanced performance of the structured catalysts can be attributed not only to good catalyst dispersion, but also to a better mass and heat transfer phenomena promoted by the foam tortuosity.

Justification for acceptance

Ceramic foams represent a very promising type of structured catalyst carriers in comparison with monoliths. High radial and axial heat transfers provided by 3D open-cell structure of foams make them suitable for exothermic reactions, namely for VOCs combustion. This work confirms that good catalytic properties, for toluene combustion, are achieved with metal based zeolites supported on cordierite foams.

TAILOR-MADE RETICULAR CORDIERITE FOAMS MANUFACTURED BY A DIRECT FOAMING PROCESS

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Recently, reticular ceramic foams have attracted much attention due to their intrinsic properties, such as high permeability, low density, high tortuosity, and low thermal mass. These characteristics are required for applications where the transport of a fluid is involved, such as filters for molten metals, hot gases, and as catalyst supports. For these applications, different foam properties are required, depending not only on the ceramic material itself, but also on the structural features of the foam. As a result, a wide range of processing routes appeared, since no process is versatile enough to fulfil all these possible foam's characteristics. In this work, a direct foaming method is proposed to produce reticular cordierite foams. Cordierite has been selected owing to its low thermal expansion, good thermal shock resistance, and a reasonable mechanical strength, making it suitable for aggressive environment applications. The method consists in dispersing ceramic particles between two separate components, an isocyanate and a polyol resin (mixture of a polyol, surfactant, catalyst and a blowing agent). The subsequent mixing of these two components leads to the formation of a polyurethane/ ceramic foam. The polymer phase is then burnt out under controlled conditions, followed by sintering to yield a highly porous ceramic foam. Some of the experimental parameters play an important role on the resulting foam properties. For instance, a good stabilization of the gas bubbles in the ceramic medium, before setting takes place, is crucial to achieve open-cell foams. Thus, the selection of the surfactant showed to be essential to the stabilization of liquid-gas interface, together with the catalyst, which rules the setting. The resulting cordierite foams present an open-cell structure, characterized by a three-dimensional array of dense struts with polyhedral cells. Their porosities are higher than 90%, with densities as low as 130 kg m^{-3}. This may limit its applicability since the resulting mechanical strength is rather low. Nonetheless, stronger and denser foams can be obtained by dipping the resulted ceramic foams within a ceramic precursor slurry (dip-coating method). Foams with densities as high as 500 kg m^{-3}, porosities around 85% and having cell sizes ranging

from 500 to 400 µm were produced. These foams also show a typical brittle behavior when submitted to compressive tests, with strengths as high as 1 MPa. The ultimate goal of this work is to fabricate metal-zeolites coated supports suitable for the catalytic combustion of volatile organic compounds.

REACTIVITY STUDIES IN BINARY AND TERNARY MIXTURES INVOLVING METHANOL, 1-PROPANOL, ACETONITRILE AND FORMAMIDE

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The linear solvation energy relationships' approach (LSER) is based on the premise that the Gibbs energy of activation can be divided into several additive energetic contributions. These contributions result from different molecular interaction mechanisms in solution that either stabilize or destabilize the initial and/or the transition state of the underlying processes.

This methodology has been extensively used in the study of solvent effects, namely in correlations between rate constants and solvents descriptors through model equations such as the TAKA equation.

In the sequence of previous work, we now present rate constants values at 25.00°C, for the heterolysis of 2-bromo-2-methylpropane in a total of 116 mole fractions corresponding to binary and ternary combinations of methanol, 1-propanol, acetonitrile and formamide.

The maximum wavelengths of 4-nitroanisole, N,N-dimethyl-4-nitroaniline, 4-nitrophenol, 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 minimization of collinearity among solvent descriptors, associated with a proper choice of training and test sets, the use of accurate statistical criteria and of external validation procedures, lead to a reliable analysis of solvent effects in these reaction processes. A comparison with previous results obtained for pure solvents was also performed.

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SUPERCRITICAL FLUID EXTRACTION OF COMPOUNDS FROM CORIANDER SEEDS: EXPERIMENTS AND MODELLING

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Livro de Resumos do 11th European Meeting on Supercritical Fluids, Barcelona, (Spain), 4-7 Maio de 2008.

Supercritical fluid extraction of the volatile and non-volatile fractions from coriander seeds was carried out under different conditions of pressure (90, 100 and 250bar), temperature (40 and 50°C), mean particle size (0.4, 0.6 and 0.8 mm) and CO_2 flow rate ($2.19x10^{-4}$, $3.05x10^{-4}$ and $4.54x10^{-4}$kg/s) to understand the influence of the process parameters on the composition and extraction yield of the oil fractions. The best extraction conditions for volatile oil were at 90bar, 40°C, 0.6 mm and $3.05x10^{-4}$kg/s and for the non-volatile oil 250bar, 40°C, 0.6 mm and $3.05x10^{-4}$kg/s (after the removal of the volatile oil).
A model based on the concept of broken and intact cells was applied to the supercritical CO_2 extraction of the volatile oil. A good agreement was obtained between the model and our experimental measurements. Moreover, a comparative evaluation of the antioxidant activity of the SFE extracts, of the essential oil (Hydrodistillation) and Soxhlet extract obtained with pentane, after deodorization, was performed using the 2,2-diphenyl-1-picrylhydrazyl method (DPPH).

MEASUREMENT AND CORRELATION OF SOLUBILITY OF RED 153 IN SUPERCRITICAL CARBON DIOXIDE

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Solubility measurements of red 153 in supercritical carbon dioxide were carried out in a flow type apparatus, at the temperature range from 323 to 393 K and for pressures from 15 to 40 MPa. The dynamic apparatus consists of the usual three sections of compression, equilibrium and expansion but some modifications have been introduced. The supercritical fluid mixture including the dye was released at the expansion valve and the dye was trapped in a system of filters without organic solvents. The dye precipitated in the system during the depressurization was recovered by washing out with methanol and analyzed in a UV-Vis spectrophotometer. The values of solubility change from 9.35×10^{-7} to 3.71×10^{-5}. Semi empirical density-based models were used to correlate the solubility of red 153 in supercritical carbon dioxide. From the correlation results, the head of red 153-CO_2 solvation and that of solute dye vaporization were determined and compared with the results in literature.

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SOLUBILITY OF ACETAMIDE AND ACRYLAMIDE IN SUPERCRITICAL CARBON DIOXIDE

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The solubilities of acetamide and acrylamide in supercritical carbon dioxide (SC-CO_2) were measured at T = (308.2, 318.2, and 333.2) K over the pressure range from (9.0 to 40.0) MPa by a flow type apparatus. The solubility of acetamide (2.3×10^{-4} to 31.3×10^{-4}) in the overall region of measurements is approximately twice that of the acrylamide (1.2×10^{-4} to 16.3×10^{-4}). The increase of pressure increases the solubility of the components and the relative location of the crossover region is observed at 12.0 MPa.
Furthermore, the experimental data were correlated by using the Soave-Redlich-Kwong cubic equation of state (SRK EoS) with the one--fluid van der Waals mixing rules.

MEASUREMENT AND CORRELATION OF SOLUBILITY OF QUINIZARIN AND 1-METHYLAMINE) ANTHRAQUINONE IN SUPERCRITICAL CARBON DIOXIDE

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Solubility measurements of Quinizarin (1,4-Dihydroxyanthraquinone) and Disperse Red 9 (1-(Methylamine)anthraquinone) in supercritical carbon dioxide were carried out in a flow type apparatus, at the temperature range from 333.2 to 393.2 K and for pressures from 12.0 to 40.0 MPa. The supercritical fluid mixture including the dye was released at the expansion valve and the dye was trapped in a system of filters without organic solvents. The dye precipitated in the system during the depressurization was recovered by washing out with ethanol and analyzed in a UV-Vis spectrophotometer. The values of solubility change from 1.43×10^{-6} to 3.16×10^{-4} to Disperse Red 9 and from 2.98×10^{-6} to 2.87×10^{-4} to Quinizarin. Semi empirical density-based models will be used to correlate the solubility of booth dyes in supercritical carbon dioxide. From the correlation results, the head of dye--CO_2 solvation and that of solute dye vaporization can be calculated and compared with the results in literature.

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THE USE OF SUPERCRITICAL FLUIDS FOR SELECTIVE EXTRACTION OF VOLATILE COMPOUNDS, SATUREJA MONTANA: A CASE-STUDY

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The performance of conventional extraction techniques (hydrodistillation and soxhlet extraction) was compared with that of the supercritical fluid extraction for the case of extracts from Satureja montana. Both volatile and non-volatile fractions were analysed by DPPH and Rancimat methods to assess their antioxidant activities. A good correlation was achieved between these two methods, indicating that the extracts were able to scavenge free radicals and to inhibit lipid oxidation. The volatile oil (obtained by supercritical fluid extraction at 90 bar and 40°C) was the most effective extract, presenting the lowest EC50 (0.06g/l) and the highest protector factor (2.03). These results demonstrated that the SFE presents advantages when compared with conventional extraction techniques, since the thermal degradation of the isolated compounds is avoided, resulting in an enhanced extract. Furthermore, the volatile oil is richer in thymoquinone than the essential oil (isolated by hydrodistillation), being this component 10 times more concentrated in the extract obtained by supercritical fluid extraction. This compound is of great importance due to its activities as antioxidant, neuroprotective and anti-cancer. The composition of the supercritical extract in carvacrol, thymol and thymoquinone may be responsible for the increase in the antioxidant activity comparing with that obtained by hydrodistillation. These results clearly show that, in this case, SFE adds value to the final product and, therefore, justify its application.

VOLUMETRIC PROPERTIES FOR THE TERNARY MIXTURE METHANOL-FORMAMIDE-ACETONITRILE

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Several chemical industrial processes use mixtures of organic solvents, and a significant number of these mixtures are non-ideal. The optimization and adequate design of equipment are conditioned by the correct assessment of the mixing properties of these mixtures. The mixing properties and their corresponding derived values are also of primary interest for theo-retical purposes namely for model development, estimation of parameters, etc.

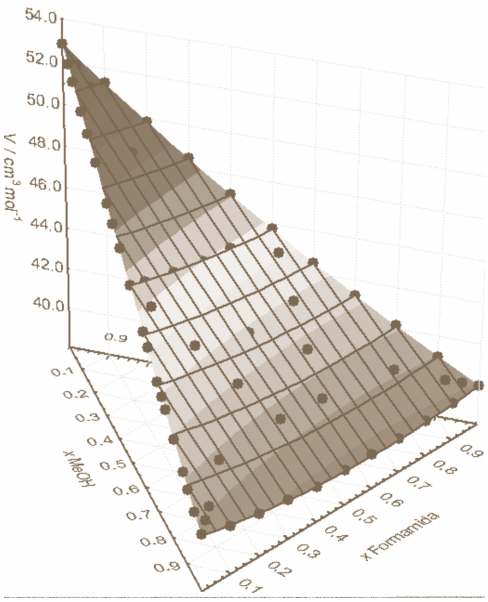

Figure 1. Molar volume for the ternary mixture methanol-formamide-acetonitrile

Following previous studies on characterization of solvent mixtures (Leitão, 2002), in this work we present molar volumes/densities' values for the ternary mixture methanol-formamide-acetonitrile.

The densities were determined in an Anton-Paar density meter (cell unit DMA 512, processing unit DMA 60 and temperature unit DT 100-30), and obtained, at 298.15 ± 0.01 K, for a total of 61 molar fractions including ternary, binary and pure solvents.

Derived properties such as the excess molar volume and the partial molar volume (Lepori, 1998) were also calculated allowing the identification of the various molecular interactions among the different solvents. The experimental values of the volumetric properties were adjusted by the Redlich-Kister (Redlich, 1948) and Cibulka (Cibulka, 1982) equations leading to a complete description of the ternary surface.

CORK PROCESSING WASTEWATER TREATMENT/VALORISATION BY NANOFILTRATION

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Livros de Resumos da Conferência "Membrane Technologies in Water and Waste Water Treatment" - IWA Regional Conference, Moscovo, Rússia, 2 - 4 de Junho de 2008.

Nanofiltration process for the treatment/valorisation of cork processing wastewaters was studied. A DS-5 DK 20/40 (GE Water Technologies) nanofiltration membrane/module was used, having 2.09 m^2 of surface area.
Hydraulic permeability was determined with pure water and the result was 5.2 $L.h^{-1}.m^{-2}.bar^{-1}$. The membrane presents a rejection of 51% and 99% for NaCl and $MgSO_4$ salts, respectively.
Two different types of regimes were used in the wastewaters filtration process, total recycling mode and concentration mode. The first filtration regime showed that the most favourable working transmembrane pressure was 7 bar working at 25°C. For the concentration mode experiments it was observed a 30% decline of the permeate fluxes when a volumetric concentration factor of 5 was reached. The permeate COD, BOD_5, colour and TOC rejection values remained well above the 90% value.
The permeate characterization showed that it cannot be directly discharged to the environment as it does not fulfil the values of the Portuguese discharge legislation. However, the permeate stream can be recycled to the process (boiling tanks) or if wastewater discharge is envisaged we have observed that the permeate biodegradability is higher than 0.5 which renders conventional treatments feasible.

ASSESMENT OF LEATHER TANNING USING CORK TANNINS CONCENTRATED BY NANOFILTRATION

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The cork processing wastewater is a very complex mixture of vegetal extracts and have, among other natural compounds, a very high content of phenolic/tannic colloidal matter, which is responsible for severe environmental problems. In the present work, the concentration of this wastewater by nanofiltration was investigated with the aim of producing a cork tannin concentrate to be utilized in tanning.

The permeation results showed that the permeate fluxes are controlled by both osmotic pressure and fouling/gel layer phenomena leading to a rapid decrease of permeate fluxes with the concentration factor.

The rejection coefficients to organic matter were higher than 95%, indicating that nanofiltration has a very good ability to concentrate the tannins and produce a permeate stream depleted from organic matter. The cork tannin concentrate obtained by nanofiltration and evaporation had a total solids concentration of 34.8 g/l.

The skins tanned by this concentrate were effectively converted to leather with a shrinking temperature of 71ºC.

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04

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

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The present work proposes the optimisation of an integrated process that consists in the coupling of Nanofiltration (NF) with Steam Stripping for the treatment of ammoniacal wastewaters contaminated by cyanides ions and phenols. These wastewaters are fractionated by NF into an ammonium concentrate and an ion-containing permeate stream. The concentrates are further fractionated in the steam stripping column.
The NF experiments were performed with a DSS plate and frame Lab-Unit 20, equipped with a HR-98-PP membrane. The NF experiments were run in concentration mode to optimise the concentrate ammonium content/permeate flux as a function of water recovery ratio (*RR*).
The optimisation of the NF/steam stripping integrated process was carried out with a sequential process simulator.
The optimisation study showed that the NF should work at a recovery ratio of 40%. At this RR the ammonium can be efficiently concentrated and purified from cyanides at reasonable permeate flow rates. The column steam consumption was also optimised as a function of the NF concentrates flowrate. The integrated process leads to an increase of the stripping efficiency and to significant energy savings.

PRODUÇÃO DE PADRÕES PARA ANÁLISE DE METAIS PESADOS EM AEROSSÓIS

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Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, FEUP, Porto, Junho de 2008.

A presença de aerossóis na atmosfera, nomeadamente em ambiente urbano, é um factor de grande influência para a saúde pública, para o clima e mesmo para a visibilidade. Conhecer a composição destes aerossóis é um factor determinante para o estabelecimento de relações entre as fontes emissoras e qualidade do ar bem como para a adequação de medidas de minimização e protecção das populações. Neste contexto o nosso grupo de investigação desenvolve metodologias de análise de aerossóis visando a sua caracterização, nomeadamente o seu teor em metais pesados. A análise de metais pesados em aerossóis pode ser realizada por digestão dos filtros em meio ácido seguida de determinação dos metais através de espectroscopia de absorção atómica. O procedimento de digestão é realizado através de processo clássico ou utilizando processos de aceleração como a extracção assistida por microondas. Novos procedimentos, nomeadamente os processos de produção de padrões de controlo e o processo acelerado de digestão, necessitam de ser validados para se efectuar análises de rotina. A validação poderia ser realizada recorrendo a padrões certificados, como por exemplo o SRM-2783 (Air Particulate on Filter) do NIST mas o seu preço elevado é o grande inconveniente para uso frequente.

Neste trabalho ensaiou-se contaminação de filtros de papel Whatman n.º 41 de 47 mm de diâmetro, habitualmente usados na recolha de aerossóis, com soluções de Pb, Cd, Cu, Cr e Ni a nível de de ppb. Estes são metais geralmente presentes em aerossóis urbanos sendo bem conhecidos os seus efeitos prejudiciais na saúde humana. Os filtros foram contaminados com soluções padrão produzidas a partir de padrões *Certipur* da Merck. Todo o material foi sujeito a descontaminação prévia utilizando ácidos *Suprapur* da Merck, ácidos com os quais também se realizou a digestão acelerada dos filtros através de microondas. Os teores de metais foram determinados por espectroscopia de absorção atómica com câmara de grafite (GFAAS). Utilizou-se o método da recta de calibração com controlo de qualidade e validação da mesma, realizado através de padrões de controlo. Os resultados obtidos mostram uma recuperação média de 97%, validando a aplicabilidade deste procedimento sequencial de contaminação e digestão para a produção de padrões de filtros contaminados com teores vestigiais de metais.

DETERMINAÇÃO DE METAIS PESADOS EM COSMÉTICOS

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Publicado em:
Livros de Resumos do XXI Encontro Nacional da Sociedade Portuguesa de Química, FEUP, Porto, Junho de 2008.

A utilização de pinturas faciais, nomeadamente nos olhos, remonta aos primórdios da existência humana. Uma das primeiras sombras conhecidas foi o minério verde malaquite $Cu_2CO_3(OH)_2$ usado desde o ano 5000 aC. As mulheres egípcias usavam trisulfureto de antimónio (Sb_2S_3) moído para escurecerem os seus olhos [1]. Nos países árabes e em África é ainda comum o uso de kohl ou surma, uma perigosa sombra para olhos em cuja composição é predominante o sulfureto de chumbo [2]. Por seu lado, em Portugal assiste-se sem controlo oficial, à comercialização de uma profusão de produtos de origem no extremo oriente, entre eles os cosméticos.

	Chumbo	Cádmio	Níquel	Crómio
Sombra	++	+	++++	++++
Blush	+	+	+	++
Batom	+			+
Rímel	+	+		++
Bronzeador	+			+

Tabela 1. Resultados qualitativos

Neste trabalho procedeu-se à análise de chumbo, cádmio, níquel e crómio em diversas amostras de cosméticos de diversas origens e diversos tipos. As amostras foram digeridas em meio ácido através de digestão assistida por microondas ou por calcinação seguida de solubilização em meio ácido. Este segundo procedimento foi utilizado em amostras com um elevado teor de gordura como os batons. As análises foram realizadas num espectrómetro de absorção atómica com câmara de grafite. Usaram-se padrões Merck Certipur para aferição dos resultados e os ácidos utilizados nas digestões foram Merck Suprapur. Os procedimentos analíticos foram realizados de acordo com as boas práticas da análise química.
Os resultados são resumidos qualitativamente na tabela 1 e mostram a presença de chumbo em todos os produtos analisados. Os maiores

teores encontrados referem-se ao crómio, com um valor máximo detectado de 293 mg/kg. O valor máximo detectado para o níquel observou-se em sombras com 199 mg/kg. Este é um valor preocupante atendendo ao alargado espectro alergénico deste metal e ao local particularmente sensível (pálpebra) onde estes produtos são aplicados. O desenvolvimento de técnicas analíticas para a análise rotineira destes produtos mostra-se assim necessária para garantia da saúde pública, embora seja dificultado pela variedade e secretismo da composição dos cosméticos [3].

POISONOUS METALS IN VEGETABLES GREW IN URBAN AREAS

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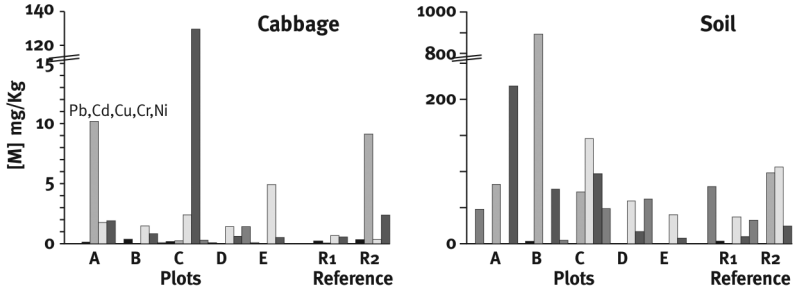
Nowadays in Lisbon city is frequent to verify the existence of small areas of agricultural exploration (vegetable gardens) in the shelving of roads with high automobile traffic intensity. In these small vegetable gardens a significant variety of species is cultivated for consuming and is usually explored by population with weak economical resources, namelly emigrants and aged retired people. These people think they are consuming healthy products, free from any chemical agents, when in reality the levels of poisonous metals and other pollutants can represent a risk [1,2]. Same countries like Portugal, Spain, UK, France, Nederlands have official programs of social vegetable gardens in several cities. The main objectives of these programs are to increment the consume of vegetables by the population where as helplessness terrains are used.

In this work we analize the most comun vegetable present in the vegetable plots in Lisbon: the gallician cabbage (*brassica oleracea*). Wa have analised five plots near the principal traffic routes of access to Lisbon and in each plot we have grab, from 25 diferent plants, the major leaf of each. In the same plot the soils are also analysed. For the gathering of three samples of soil in each plot, and in a random way, a plastic tube with 4 cm of diameter and 25 cm deep are used. The samples after proper treatment were digested with *Suprapur* acids from Merck in a micro-wave digestion system from CEM. The contend of metals in the samples were determined by GFAAS (Graphite Furnace Atomic Absorption Spectrometry) using a spectrometer Thermo, model Solaar.

The results of metal contend in cabbage and soils are shown in the figure below.



The values obtained are below the maximum defined in the Codex Alimentarius but some are much closed to the recommended maximum. Therefore the exploration of vegetable gardens in urban areas, near roads with intensive car traffic [3], needs to be controlled periodically to preserve the health of their consumers.

CALIX[4]ARENES FOR MEMBRANE ION-SELECTIVE ELECTRODES

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Calixarenes are synthetic cyclic oligomer macromolecules formed by phenolic rings, bonded by methylene bridges[1,2]. These compounds have intramolecular cavities, in "basket" form, which enable occlusion interactions with other molecular species, ions and other macromolecules (Fig. 1).

Calixarenes have high fusion temperatures, are insoluble in water and in the majority of organic solvents. In terms of Calixarenes applications some can be stressed out, such as: extraction of several pollutants present in aqueous matrixes, construction of membranes for chemical and biochemical sensors, chromatographic support, adsorbent, biomedical monitorization, selectivity and extraction of heavy metals present in several types of matrixes [3].

In this paper, we report the construction and the evaluation of a ion--selective electrode based on p-tertbutilcalix[4]arene or tetrapy-ridyl-calix [4]arene in polymeric membranes of PVC. The membranes are optimized in composition attending the components: PVC, ionophores, plasticizers, potassium tetrakis(4-chlorophenyl)borate and the solvent (THF) quantity.y

For the measurement of the performance and selectivity of the electrode, an internal reference electrode of Ag/AgCl with a filling solution of MCl_2 0.01 M has been used [4]. M is the metal under study. The external reference electrode was an AgCl/Ag electrode with KCl (saturated). A cell assembly of the following type was used:

Ag/AgCl | 0.01 M MCl_2 | PVC membrane | sample solution | KCl (saturated) | AgCl/Ag.

The electrode response shows a linear behavior toward Pb^{2+} ion with 10^{-6} M to 10^{-3} M of a linear range. The selectivity coefficients for other tested cations were low for a future analytical use. However, the response time of this electrode is high for practical uses.

We continue to develop these electrode systems with other calix[4] arene membranes and other filling solutions of the internal reference electrode. The configuration of the membrane was also altered.

SOLAR ACTIVITY AND FOREST FIRES

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The number of forest fires as well as surfaces they occupy has increased from year to year. Difficult which has existed during the research relates to modest database. Unsuccessful was the attempt to unite necessary satellite data with data on fires for period 1991-2001. That is why it was decided to add FAO UN results to establish whether there is a signal of the eventual causality. Proceeding from the official data, the cause for about 43% of the forest fires was not established. The monograph points out the hypothetic possibility that certain processes on the Sun could be the explanation. Depending on solar wind parameters, the differences concerning the regional development of the weather conditions seem to give a universal approach in the only possible way for now. On the basis of the researches showed in this study, we may conclude the following:

| in all cases the data were gathered for, up to several days earlier the coronary holes and energetic regions in geoeffective position on the Sun had preceded forest fires in Europe. In every concrete situation, the emission of strong electromagnetic and thermal corpuscular energy from these sources had preceded fires;

| basic ways of solar wind penetration into the magnetosphere are a) reconnection (in the area of geomagnetic poles) and b) direct solar wind penetration under the dominant effect of the kinetic energy (near geomagnetic anomalies);

| solar wind directed towards the Earth gets weaker with deeper and deeper penetration towards the topographic surface. The modifications happening above the Atlantic anomaly and over magnetosphere tropics also represent the border area modern science has come to;

| air masses seized by power stream of the solar wind particles, are subject to the magnetic field laws and their moving is on the account of particles' energy of the power stream;

| geomagnetic coordinates can represent the basis for mathematical

equation usage, which describe the trajectories of air mass movements;

| the direction of air mass movements is determined by the polarization of the solar wind charged particles. In the northern hemisphere, the movement of winds made on the account of the proton solar wind energetic particles has the left direction. Wind speed increases with the height increase and it is directly proportional to the kinetic energy of the solar wind particles' increase;

| cloudiness represents one of the most important factors, determining whether charged particles will be deposited to the topographic surface;

| on basis of the preliminary results, there are indications that the cosmic radiation (especially in period of reduced solar activity) may also cause fire phenomenon. As already said, the cosmic radiation in certain situations may be characterized by far higher temperatures, speeds, particle density, that is, by far stronger electromagnetic waves than ever measured for the solar wind. "However, the physical mechanism of solar activity effects on weather phenomena remains unclear. It is suggested that a significant part in the transfer of the solar variability to the lower atmosphere may be played by charged particles of solar and galactic origin, mainly protons, with energies from around 100 MeV to several GeV.

WASTE MANAGEMENT AND THE ENVIRONMENT IV

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Acrylamide is an amide with potentially hazardous effects on environment and human health. Humans exposed to acrylamide have revealed symptoms such as muscular weakness, skin and mucous irritation, nausea and numbness. In addition acrylamide is a potent neurotoxin that can cause serious nervous system damage. Long term exposure to this chemical may also be responsible for several types of cancer.

Environmental effects may include death of animals, birds and fish, and death or low growth rate in plants. Accumulation in groundwater may also occur, as well as persistence in aquatic environments [1, 2]

Acrylamide is mainly used in the production of water-soluble polymers used as additives for drinking water, in enhanced oil recovery, in wastepaper recycling, as soil conditioning agents, in sewage and waste treatment, in the synthesis of dyes, in textile industry, as copolymers for contact lenses and in the construction of dam foundations, tunnels, and sewers.

On the other hand acrylamide forms in certain foods, particularly plant-based foods that are rich in carbohydrates and low in protein, during processing or cooking at high temperatures.

Like acrylamide, formamide is an amide that may pose serious environmental and human health effects. In this regard it is essential to develop methods in order to determine, reduce and control the amount of acrylamide and/or formamide present in the environment, namely wastewater [3], as well as in food, human and animal organisms.

Our group has been working in the development of a potentiometric biosensor [5] in order to determine the amount of these amides in environmental and food samples. The biosystem consists in whole cells of *Pseudomonas aeruginosa* containing intracellular amidase activity instead of the traditional use of cellular extract. In the construction of the biosensor, the cells are immobilized [5] on the surface of

a polyethersulphone membrane in the presence of glutaraldehyde as bifunctional reagent. This membrane is then attached to the surface of an ammonium ion selective electrode [6].The reaction that occurs is the hydrolysis of formamide or acrylamide (catalyzed by amidase), with formation of formic or acrylic acid, respectively, and ammonium ion which is potentiometric measured by the ammonium ion selective electrode.

The results obtained revealed excellent analytical characteristics of the biosensor such as linear concentration range for formamide and acrylamide, sensitivity, repeatability, response time and stability, for synthetic as well as for real environmental samples, namely waste-water samples. Furthermore the half-life time of the biosensor obtained for acrylamide was about 18 days. Presently our investigation aims the optimization of the biosensor half-life time for acrylamide as well as for formamide.

PROCESSO PARA A DEPURAÇÃO E RECUPERAÇÃO DO GÁS FORMADO EM FORNOS DE CARBONIZAÇÃO DE MADEIRA

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Patente Número: PT 103636
Data de Apresentação Nacional: 8 de Janeiro de 2007
Data de Publicação: 18 de Janeiro de 2008

O presente invento diz respeito a um processo de depuração e recuperação do gás formado em fornos de carbonização de madeira em processos de produção de carvão vegetal. Do ponto de vista ambiental o processo de carbonização de madeira é consideravelmente poluente lançando para a atmosfera um gás com elevado teor poluente, cuja toxicidade na atmosfera se encontra bem documentada. O processos que se descreve é adequado para a depuração física e química dos gases de exaustão formados, permitindo ainda a sua recuperação como combustível (visto ser um gás de baixo poder calorífico) sendo mínima, ou quase nula, a quantidade lançada para a atmosfera. Este invento compreende as seguintes operações: recolha do gás, remoção de partículas sólidas, remoção de líquidos arrastados, transporte e armazenagem do gás.

PROCESS OF CORK PRE-EXPANSION BY SUBMISSION TO MICROWAVE RADIATION AND RESULTING PRODUCT THEREOF

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Patente Número: WO 2008/115086 A1
Data de Apresentação Internacional: 20 de Março 2008
Data de Publicação: 25 de Setembro de 2008

This invention relates to a process, and to the resulting material, that allows the volumetric expansion of cork without using substances foreign to the cork system. More precisely, it relates to a process that consists in submitting cork to microwave radiation, obtaining a more bulky material and consequently increasing its yield and reducing its specific weight.

NOVOS COMPLEXOS DE RÉNIO COM PIRAZOLE OU TRIS(1-PIRAZOLIL) METANOS E SUA APLICAÇÃO COMO CATALISADORES DA OXIDAÇÃO PARCIAL, EM CONDIÇÕES SUAVES, DE ETANO A ÁCIDO ACÉTICO E ACETALDEÍDO E DE CICLO-HEXANO A CICLO-HEXANOL E CICLO-HEXANONA

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Patente Número: PT103735
Data de Publicação: 8 de Abril de 2008

A invenção refere-se a novos complexos de rénio com pirazole ou tris(1-pirazolil)metanos, de fórmulas (1) a (4), e ao uso daqueles compostos e de complexos relacionáveis como catalisadores (i) da oxidação parcial do etano a ácido acético, (ii) da oxidação parcial do etano a acetaldeído e (iii) da oxidação parcial peroxidativa do ciclo-hexano a ciclo-hexanol e ciclo-hexanona, todos os processos realizados em condições suaves e com elevados rendimento e selectividade. A invenção refere-se ainda ao uso vantajoso de microondas na síntese daqueles complexos.

UTILIZAÇÃO DE DERIVADOS DE CALIXARENOS NO ISOLAMENTO DE PROTEÍNAS E BIOCATÁLISE EM SOLVENTES ORGÂNICOS

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Mestrado em: Química Analítica Aplicada
Grau Concedido por: Faculdade de Ciências da Universidade de Lisboa
Orientadores: Professor Doutor Amin Karmali e
Professora Doutora Maria Luísa Serralheiro
Provas Concluídas em: 28 de Fevereiro de 2008

Neste trabalho foram utilizados ácidos carboxílicos derivados de *p-tert*-butilcalix[4,6,8]areno na extracção selectiva de duas proteínas: a mioglobina e a hemoglobina. Os três calixarenos apresentaram a capacidade de extrair as proteínas para a fase orgânica, com parâmetros de extracção superiores a 0,90.
Estas proteínas demonstraram pseudoactividade de peroxidase na reacção de oxidação da seringaldazina na presença de peróxido de hidrogénio, quer em meio aquoso quer em meio orgânico usando o derivado ácido de *p-tert*-butilcalix[6]areno em clorofórmio. A biocatálise destas duas proteínas foi investigada variando os seguintes parâmetros: pH, concentração da proteína e do substrato.
A actividade específica máxima da mioglobina foi determinada em meios aquoso e orgânico obtendo-se os valores de 1,08 x 10^{-1} e 1,37 x 10^{-1} U.mg proteína^{-1} a pH inicial de 6,5, respectivamente. A hemoglobina apresentou em meio aquoso actividade específica máxima de 1,04 U. mg proteína^{-1} a pH 5,5 e em meio orgânico de 9,92 x 10^{-2} U.mg de proteína^{-1}, a pH inicial de 7,5.
Os parâmetros cinéticos em meio aquoso ($V_{máx}$, K_m, k_{cat} e k_{cat}/K_m) foram determinados em função do pH, assim como os parâmetros cinéticos aparentes ($V'_{máx}$, K'_m, k'_{cat} e k'_{cat}/K'_m) em meio orgânico.
A estabilidade do complexo proteína-calixareno foi analisada para ambas as proteínas em função do pH inicial tendo-se obtido valores de $t_{1/2}$ na gama de 2 – 5 dias. Os complexos proteína-calixareno no meio orgânico foram recuperados para soluções aquosas frescas alcalinas, com valores de recuperação da pseudoactividade de peroxidase superiores a 100%.
O derivado ácido de *p-tert*-butilcalix[6]areno foi utilizado na extracção da hemoglobina a partir de sangue humano obtendo-se um valor de 0,50 para o parâmetro de extracção. A proteína foi purificada a partir de sangue humano usando uma matriz cromatográfica de um polímero contendo unidades de *p-tert*-butilcalix[6]areno na forma ácida, com um rendimento final de pseudoactividade da hemoglobina de 34,42% e um factor de purificação de 12. A análise electroforética da preparação purificada da hemoglobina revelou uma banda de proteína com Mr de 61 kDa em PAGE nativa que foi coincidente com a banda de pseudoactividade de peroxidase *in situ*.

PROJECTO E CONSTRUÇÃO DE UM PILOTO DE DESTILAÇÃO CONTÍNUA. ESTUDO DA SUA MANUTIBILIDADE

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Grau Concedido por: Faculdade de Engenharia da Universidade do Porto
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Provas Concluídas em: 11 de Novembro de 2008

As colunas de destilação são dos equipamentos mais utilizados na indústria para a realização de processos de separação. Perturbações durante o seu funcionamento, como a avaria de componentes podem resultar num desvio ao normal funcionamento da instalação. Um estudo desenvolvido por *Kister1* (2003) mostra que o número de avarias em colunas de destilação não está a diminuir, mas sim a aumentar.
O objectivo do presente trabalho, foi desenvolver uma análise de falhas e seus efeitos (FMEA) a uma coluna de destilação contínua piloto do Laboratório de Tecnologia Química do ISEL. A instalação completa é constituída pela coluna de destilação, pela unidade de aquisição e controlo (UAC) e pela estrutura de suporte. A instalação tem uma altura de 3,7 m; 1,0 m de largura na base; 0,5 m de largura no topo e 0,5 m de profundidade. Na sua totalidade a instalação é constituída por 326 componentes de diversos materiais: vidro *Duran*®/Borosilicato3.3; liga de aluminínio-silício, aço inoxidável; *Teflon*; plástico e Quartzo.
Da análise FMEA desenvolvida, identificou-se:
| 726 modos de falha que originaram 942 efeitos dos modos de falha;
| Que 88,4% dos modos de falha identificados possuem uma probabilidade deocorrência "Muito Improvável;
| Os subsistemas ebulição e estrutura possuem a maioria dos modos de falha do equipamento, cerca de 59% (subsistema ebulição 35%, subsistema estrutura 24%);
| Que 43% dos efeitos dos modos de falha possuem uma severidade "Muito Crítico", 34,3% "Crítico" e 22,3% "Pouco Crítico";
| Que no subsistema estrutura e no subsistema unidade de aquisição e controlo o grau de severidade predominante é o mais severo, com 98,2% e 66,7% respectivamente;
| Que na instalação existem 14% de modos de falha críticos e que destes 4,6% localizam-se no subsistema ebulição e 4,5% no subsistema unidade de aquisição e controlo.
Como continuação deste trabalho, seria interessante a monitorização das falhas ocorridas nesta instalação e a optimização da base de dados desenvolvida, de forma a facilitar a introdução de registos de

falhas ou acções de manutenção correctivas ou preventivas, para validar futuramente a análise de sensibilidade que serviu de base para a atribuição dos modos de falhas e seus efeitos a cada componente, assim como os índices de probabilidade de ocorrência e severidade atribuídos a cada modo de falha.

TÉCNICAS PREDITIVAS APLICADAS A CONTROLO DE PROCESSOS

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Provas Concluídas em: 28 de Novembro de 2009

A necessidade que as indústrias têm, hoje em dia, de lidar com processos cada vez mais complexos, onde a quantidade de variáveis a controlar e restrições processuais a impor aumentou exponencialmente nas últimas décadas. Uma maior competitividade e eficiência, lado-a-lado com a redução de custos, proporcionou à comunidade científica e industrial explorar mais profundamente o controlo de processos, com vista à construção de técnicas avançadas para fazer face a estas exigências.
O controlo preditivo baseado em modelos - MPC - engloba diversas classes de controladores que utilizam algoritmos de predição/previsão e modelos matemáticos representativos do sistema, que juntamente com restrições processuais permitem operar junto de referências e tornar o controlo mais eficiente e seguro.
O sucesso do MPC nos sistemas lineares com restrições deve-se, sobretudo, ao facto de reduzir o problema de optimização a um problema de programação quadrática, de fácil implementação e resolução. Além do mais, trata-se de um tipo de controlo bastante mais flexível e, ao mesmo tempo, mais robusto que o controlo clássico ou convencional, já que pode lidar com processos multivariáveis sem precisar de alterações significativas na sua construção.
Neste trabalho aplicam-se técnicas de controlo preditivo a processos não lineares multivariáveis. Estuda-se, ainda, o desempenho desta classe de controladores comparando-a com técnicas de controlo convencional. Nomeadamente, estuda-se um sistema de três tanques em série em que o caudal é manipulado através de válvulas com característica não linear. O processo é modelado através de princípios de conservação e é validado por um conjunto real de ensaios que permitiu, ainda, obter experimentalmente a característica das válvulas.
O modelo validado permitiu desenvolver um controlador preditivo multivariável para controlar os níveis da instalação. Demonstra-se que os controladores preditivos apresentam grandes vantagens em relação ao controlo clássico com malhas independentes.

VISCOSIDADE E DENSIDADE DE FLUIDOS: MEDIDA E CORRELAÇÃO

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Provas Concluídas em: 12 de Dezembro de 2008

Esta tese tem como objectivo fundamental o desenvolvimento de programas de medida experimental de propriedades termofísicas de fluidos e o desenvolvimento de métodos de correlação e de previsão, com exactidão adequada às aplicações. O domínio científico centra-se na área da termodinâmica de fluidos aplicada à engenharia, com especial ênfase na medida experimental, interpretação, correlação e previsão das propriedades de transporte, nomeadamente, viscosidade de líquidos puros e de misturas, de grande importância para o projecto e exploração de processos de Engenharia Química.
A presente tese divide-se em três áreas: (i) realização de medidas simultâneas da viscosidade e da densidade do tolueno, e colaboração na feitura das correlações que consubstanciaram a proposta do tolueno como líquido padrão para a viscosidade, realizado sob os auspícios da sub-comissão I.2 – Propriedades de Transporte da, entretanto extinta, Comissão de Termodinâmica da IUPAC; (ii) estudo do efeito de plasticização – redução da viscosidade de polímeros – por acção da adição de fluidos supercríticos, baseado no estudo experimental de sistemas Poli(etileno)glicol saturado com CO_2 supercrítico; e (iii) medida da viscosidade de sistemas de hidrofluorcarbonetos, utilizados como refrigerantes alternativos (HFC-125, HFC-143a e R-507A), *amigos do ozono*. Foram aplicados e desenvolvidos modelos para correlacionar os dados experimentais em todos os casos estudados.

PRODUCTION, PURIFICATION AND PARTIAL CHARACTERIZATION OF SOME LIGNOCELLULOSIC ENZYMES FROM TWO STRAINS OF WHITE-ROT BASIDIOMYCETES

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Provas Concluídas em: 20 de Junho de 2008

Strains of *Pleurotus ostreatus* and *Coriolus versicolor* were grown in submerged culture with tomato pomace as sole carbon source for production of lignocellulosic enzymes. The culture of *Coriolus versicolor* exhibited a peak of laccase activity (362 U/L of fermentation broth) on the 3rd day of culture with a specific activity of 3.7 U/mg protein. On the other hand, *Pleurotus ostreatus* revealed a peak of laccase activity (147 U/L of fermentation broth) on the 4th day of culture with a specific activity of 2.8 U/mg protein. The culture of *Coriolus versicolor* exhibited a peak of xylanase activity (2565 U/ L of fermentation broth) on the 14th day of culture with a specific activity of 11.7 U/mg protein. As for *Pleurotus ostreatus*, it revealed a peak of xylanase activity (3558 U/L of fermentation broth) on the 6th day of culture with a specific activity of 16.4 U/mg protein. The culture of *Coriolus versicolor* exhibited a peak of polygalacturonase activity (1427 U/L of fermentation broth) on the 3rd day of culture with a specific activity of 14.5 U/mg protein. *Pleurotus ostreatus* revealed a peak of polygalacturonase activity (2181 U/L of fermentation broth) on the 4th day of culture with a specific activity of 42.8 U/mg protein.
Differential chromatographic behaviour of polygalacturonase, xylanase and laccase from both strains of white rot fungi were investigated on immobilized metal chelates. The enzymes revealed different affinities for immobilized metal chelates which obeys the following order: polygalacturonase › laccase › xylanase.
The effect of ligand concentration, pH, the length of spacer arm and the nature of metal ion was studied for enzyme adsorption on immobilized metal affinity chromatography (IMAC). The presence of imidazole in the equilibration buffer abolished the adsorption of the enzymes to immobilized metal chelates and it was possible to devise suitable one-step purification schemes for polygalacturonases from *Pleurotus ostreatus* and *Coriolus versicolor* and for laccases from *Coriolus versicolor*, by using a column of Sepharose 6B-EPI 30-IDA-Cu(II). For Pleurotus ostreatus, the purified polygalacturonase exhibited a specific activity of about 1600 U/mg protein, final recovery of enzyme activity of 80% and a purification factor of about 65. For

Coriolus versicolor, the purified polygalacturonase exhibited a specific activity of about 150 U/mg protein, final recovery of enzyme activity of 100% and a purification factor of about 10. Purified laccase from *Coriolus versicolor* was obtained with a specific activity of about 15.0 IU/mg protein, a final recovery of enzyme activity of about 42.7% and a purification factor of about 10.
An interesting result was obtained for laccases from *Coriolus versicolor* as, under the appropriate experimental conditions, IMAC revealed two populations of isoenzymes, one with low and the other with high pI.
An innovative one-step purification scheme for laccases from *Pleurotus ostreatus* and *Coriolus versicolor* was proposed in an affinity column using urea as affinity ligand. Elution was achieved either with $CuSO_4$ or $(NH_4)_2SO_4$. For *Pleurotus ostreatus* purification factors from 14 to 46 were achieved. Recovery of enzymatic activity was nevertheless low (about 50%). For *Coriolus versicolor*, purification factors from 4.6 to 6.0 were achieved and recoveries were in the range 70-85%. The results that were presented allow the formulation of the hypothesis that there is a specific interaction between the Cu(II) ions of the enzymes and the chromatographic support. Both electrostatic and coordination interactions are thought to play a role in this interaction.
Purified preparation of polygalacturonase from *Pleurotus ostreatus* exhibited a pH and temperature optima of activity at 7.0 and at 50°C, respectively. The kinetic parameters (Vmax, Km, Kcat, and Kcat/Km) of purified enzyme were found to be 5530.8 ± 260.7 U/mg of protein, 13.23 ± 2.79 mg/ml of polygalacturonic acid, 5553.01 ± 261.7 s^{-1} and 419.72 $s^{-1}.mg^{-1}$, respectively. Purified enzyme exhibited a half life ($t_{1/2}$) of 60 ± 7.45 min and 35 ± 0.37 min at 50°C and at pH 6.0 and 7.0, respectively. The analysis by SDS-PAGE of the purified preparation an activity band of polygalacturonase with Mr of 65 kDa. However, gel filtration chromatography of the purified enzyme exhibited a Mr value of 41.1 kDa.
Purified preparation of polygalacturonase from *Coriolus versicolor* was also analysed by SDS-PAGE, and exhibited three protein bands and three activity bands of polygalacturonase, with the main protein band exhibiting a Mr of 43 kDa.
The purified preparation of laccase from *Coriolus versicolor* exhibited an optimum pH of activity at pH 5.0, with o-dianisidine as substrate, and of 3.0 with ABTS. The optimum temperature of activity for this enzyme was found to be at 60°C in acetate buffer at pH 4.5. The thermal stability of the purified enzyme was investigated at 45 and 60°C in acetate buffer at pH 4.5 which revealed half life values ($t_{1/2}$) of 19,4 ± 2,2 hr and 0,50 ± 0.0,12 hr, respectively.
The purified preparation of laccase from *Pleurotus ostreatus* exhibited an optimum pH of activity at pH 6.0, with o-dianisidine as substrate, and of 3.0, when ABTS was used. The optimum temperature of activity for this enzyme was found to be at 45°C in acetate buffer at pH 4.5. The thermal stability of the purified enzyme was investigated

at 45°C in acetate buffer at pH 4.5 which revealed a half life value ($t_{1/2}$) of 12,49 ± 0,02 hr.
The kinetic parameters (Vmax and Km and kcat) of the purified laccases from both strains of basidiomycetes were also obtained for o-dianisidine, guaiacol and ABTS as substrates.

04

05

ENGENHARIA DE SISTEMAS DE POTÊNCIA E AUTOMAÇÃO

Anuário Científico 2008

ISEL

HIGH PRECISION HF-180 ION IMPLANTATION USING A HIGH-CURRENT ION IMPLANTER

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The development of accurate mass spectrometry, enabling the identification of all the ions extracted from the ion source and further precise ^{180}Hf isotope implantation, in a high current implanter is described. The developed spectrometry system uses two signals (x-y graphic), one proportional to the magnetic field (x-axes), taken from the high-voltage potential with an optic fiber system, and the other proportional to the beam current intensity (y-axes), taken from a beam-stop. The ion beam mass register in a mass spectrum, of all the elements magnetically analyzed with the same radius and defined by a pair of analyzing slits, as a function of their beam intensity, is presented. Hence, it is possible to implant $^{180}Hf^{+}$, with less than 1% contamination from the neighbor isotopes, in order to conduct material characterization studies by Perturbed Angular Correlations. The precision of the low dose ion implantation has been done by Neutron Activation Analysis.

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Nuclear Instruments & Methods in Physics Research section B-Beam Interactions with Materials and Atoms, Vol. 266, Issue: pp. 3661-3666, 2008.

LOW-POWER 6-bit 1-GS/s TWO-CHANNEL PIPELINED ADC WITH OPEN-LOOP AMPLIFICATION USING AMPLIFIERS WITH LOCAL-FEEDBACK

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Publicado em:
IEEE International Symposium on Circuits and Systems ISCAS'08, 2008, 2258-2261.

Wireless short range connectivity with high data rate capabilities, is and will be one of major driven technology for the consumer electronics mass market. Wireless (USB) and Ultra Wideband (UWB) Bluetooth are examples of such technologies since they start from an installed base in the billions of ports. Software radio UWB receiver implementation has numerous potential benefits ranging from low-cost and ease-of--design to flexibility. However such approach implies analogue-to-digital converters (ADCs) capable of sampling rates in order of GS/s, which constitutes a technical challenge when using a low-cost pure digital CMOS technology.

This work presents a 1.2 V 20 mW 6-bit 1GS/s 2-channel pipeline ADC designed in a 1.2 V, 130nm 1P-8M CMOS technology. In each pipelined stage, the open-loop residue amplification is carried-out by using a shared amplifier between channels. This amplifier employs local-feedback in order to achieve constant closed-loop gain against Process-Supply-Temperature (PVT) variations and thus, avoiding the need of any digital self-calibration or gain-control techniques. Time skews between the 2 channels are highly reduced, by using two passive front-end Sample-and-Hold (S/H) circuits, with dedicated switch-linearization control (SLC) circuits, driven by a single clock phase. Simulations reach a peak SNDR of 34 dB, a SFDR of 47 dB, a THD of -43 dB and 5.35-bit ENOB, for a power dissipation of 20 mW which corresponds to an energy efficiency better than 0.5 pJ per conversion. Moreover, all pipelined stages are made equal and no scaling is used which highly simplifies the layout effort.

POWER-AND-AREA EFFICIENT 14-bit 1.5 MS/s TWO-STAGE ALGORITHMIC ADC BASED ON MISMATCH--INSENSITIVE MDAC

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Sigma-Delta (∑Δ) architectures, either continuous-time (CT) or switched--capacitor (SC) can simultaneously achieve high *BW*, high resolution, and low power. Multi-bit SC implementations of ∑Δ modulators (∑ΔM) can reach *FM1* of the order of 0.5 pJ to 0.7 pJ and *FM2*=0.54 pJ.mm2 is obtained; however, the decimation filter is not taken into account. A previous CT-∑Δ realization includes the decimation filter which dissipates an additional power of 50% and occupies an area of 30% of the ∑ΔM. A high energy efficiency with *FM1*=0.3 pJ is measured, but when area is also taken into account we end up with *FM2*=2 pJmm2. The state-of-the art is that CT-∑Δ are in general, 1.5 times more energy efficient than their SC counterparts, but less area efficient.
This paper presents a 14-bit 1.5 MSample/s two-stage algorithmic ADC with a power-and-area efficiency better than 0.5 pJmm2 per conversion. This competes with the most efficient architectures available today namely, ∑Δ and self-calibrated pipeline. The 2 stages of the ADC are based on a new 1.5-bit mismatch-insensitive MDAC and simulations demonstrate that a THD of –79 dB and an ENOB better than 12 bits can be reached without self-calibration.

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IEEE International Symposium on Circuits and Systems, ISCAS'08, 2008, 220-223.

05

NEW SOLID-STATE MARX TOPOLOGY FOR BIPOLAR REPETITIVE HIGH-VOLTAGE PULSES

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Proceedings Power Electronics Specialists Conference, 2008. 15-19 June 2008 Rhodes/Greece, pp. 791-795

A novel bipolar high-voltage modulator topology, based on the Marx generator concept, is proposed for high-voltage repetitive pulsed power applications. The proposed topology is a generalized version of the negative and positive all-solid-state Marx modulator concepts, which takes advantage of the intensive use of power semiconductor switches to increase the performance of the classical circuit, strongly reducing losses and increasing the pulse repetition frequency. Additionally, the proposed topology enables the use of typical half-bridge semiconductor structures while ensuring that the maximum voltage blocked by the semiconductors is the voltage of the capacitor in each stage. Due to semiconductor topology used the output voltage is very flexible. Hence, it is possible to change from negative to positive unipolar to bipolar pulse, with different duty cycles and different switching patterns. Experimental results are presented and discussed. A laboratory prototype with 10 kW peak power, of this bipolar solid-state modulator circuit, was assembled 1200 V IGBTs and diodes, operating with 1000 V d-c input voltage and 10 kHz frequency, giving 2 kV bipolar pulses, 5 A, with 5 ms into a resistive load.

NEW REPETITIVE BIPOLAR SOLID-STATE TYPE MODULATOR

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A broad circuit topology for bipolar or unipolar high-voltage repetitive pulse power applications is proposed. This circuit constitutes a merging version of the negative and positive solid-state Marx modulator concepts, which take advantage of the intensive use of semiconductor devices to increase the performance of the classic circuit.
The flexibility of the proposed modular circuit enables the operation with negative and/or positive pulses, with different duty cycles, frequencies and relaxation times between the positive and negative pulse. Additionally, the switching topology enables the discharge of the parasitic capacitances after each pulse, allowing the use of capacitive loads.
A 60 kW peak power laboratory prototype was assembled with four stages, using 1200 V IGBTs and diodes, operating with 1000 V dc input voltage and 2 kHz frequency, giving 4 kV/15 A bipolar pulses, with 5 ms pulse width and 5 ms relaxation time into a resistive load.

Publicado em:
Proceedings 28th International Power Modulator Symposium/2008 High Voltage Workshop, 27-31 May 2008, pp. 253-256.

DIGITAL TEMPERATURE AND HUMIDITY MONITORING UNIT FOR REMOTE APPLICATIONS

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Publicado em:
Proceedings of the 12th Annual International Symposium on Consumer Electronics, IEEE-ISCE2008; 14 a 16 de Abril de 2008. ISBN: 978-1-4244-2422-1.

A digital hardware unit designed to integrate a network of digital thermometers as well as a group of analogue humidity sensors is presented. The unit was conceived to operate with low consumption as required for remote applications. The power supply is provided by a 230VAC/12VDC adapter or by internal rechargeable Ni-Cd batteries. The recorded data is stored in a 128kbyte EEPROM and can be accessed by a single RS-232C port in a desktop or laptop PC through developed software. A GSM-SMS alarm system was also integrated to warning users about critical events.

ANTI-SLIP WHEEL CONTROLLER DRIVE FOR EV USING SPEED AND TORQUE OBSERVERS

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A wheel slip controller of an electric vehicle with two independent rear wheel drives is presented. The vehicle dynamic model and the proposed torque controller for the DC motors are also presented. The speed and torque observer solution proportionate the necessary external torque estimation to the anti-slip wheel controller. The wheel slip is based on the comparison of the real vehicle velocity and the estimated velocity given by the speed observer.

Publicado em:
Proceedings of the International Conference on Electrical Machines, IEEE-ICEM'08; VilaMoura – Portugal de 6 a 9 de Setembro 2008, ISBN: 978-1-4244-0755-2;

A PHASOR SPEED CONTROL OF A SINGLE OR TWO PHASE INDUCTION MOTOR

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Publicado em:
Proceedings of the 2008 International Conference on Electrical Machines, IEEE-ICEM'08; VilaMoura – Portugal de 6 a 9 de Setembro 2008, ISBN: 978-1-4244-0755-2;

This paper is focused on the speed control of a single or two phase induction motor using a diametrical inversion (DI) of the stator voltages. The changes in the speed error sign are responsible for each DI which inverts the stator voltage phasor and its angular velocity. The main and the auxiliary windings are always connected and thus the speed error sign allows to determinate the rotating field direction. The motor is fed by a rectifier associated with a three-phase inverter. The core of the drive command it's a 16-bit dsPIC device, which receives the speed error sign and generate the appropriate PWM reference voltages signs to the three-phase inverter. Simulation and experimental results allow assume a good performance.

SPEED CONTROL OF A SINGLE AND TWO PHASE INDUCTION MOTORS USING THE DIAMETRICAL INVERSION

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The diametrical inversion (DI) of the stator voltages has been used to control the rotor position of the three-phase-induction motor. In this paper the DI is applied on a single-phase induction motor drive to control its speed. The change of the speed error sign causes a DI. Each DI inverts the stator voltage phasor and its angular velocity. The main and the auxiliary windings are always connected and so the sign of the speed error determines the rotating field direction. The motor is fed by a rectifier associated with a three-phase inverter module. Two reference voltages are PWM modulated using a sigma-delta closed loop strategy. The global system was implemented by Matlab/Simulink software. The simulation and experimental results allow assume a good performance.

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05

MICRO-GENERATION EVALUATION OF THE ZERO EMISSIONS TECHNOLOGIES IN THE PORTUGUESE MARKET

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Publicado em:
Livros de Resumos do 5th International Conference on European Electricity Markets – EEM08, Lisbon, 28-30 May 2008.

Micro-generation is the small scale production of heat and/or electricity from a low carbon source and can be a powerful driver for carbon reduction, behavior change, security of supply and economic value. The energy conversion technologies can include photovoltaic panels, micro combined heat and power, micro wind, heat pumps, solar thermal systems, fuel cells and micro hydro schemes. In this paper, a small research of the availability of the conversion apparatus and the prices for the micro wind turbines and photovoltaic systems is made and a comparison between these two technologies is performed in terms of the availability of the resource and costs. An analysis of the new legal framework published in Portugal is done to realize if the incentives to individuals' investment in sustainable and local energy production is worth for their point of view. An economic evaluation for these alternatives, accounting with the government's incentives should lead, in most cases, into attractive return rates for the investment. Apart from the attractiveness of the investment there are though other aspects that should be taken into account and those are the benefits that these choices have to us all. The idea is that micro-generation will not only make a significant direct contribution to carbon reduction targets, it will also trigger a multiplier effect in behavior change by engaging hearts and minds, and providing more efficient use of energy by householders. The diversified profile of power generation by micro-generators, both in terms of location and timing, should reduce the impact of intermittency or plant failures with significant gains for security of supply.

INDUCTION MOTOR PARAMETERS IDENTIFICATION FROM BENCH TESTS USING A NEWTON-RAPHSON METHOD

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A numerical procedure using a Newton-Raphson method for the calculation of induction motor model parameters is presented. The method, which requires a no-load and a blocked rotor test, is intended for steady state torque and efficiency evaluation of three-phase single-cage rotor induction machines within the rated range of operation. The performance of the method is analyzed in terms of speed of convergence as well as of sensitivity to measurement deviations in the essential quantities, yielding important conclusions. A comparison is also made with a corresponding procedure from IEEE-Std 112. Results obtained with motor data are presented confirming the capabilities of the presented approach.

Publicado em:
Proceedings de ICEM'08 XVIII International Conference on Electrical Machines, Vilamoura, Portugal, 6 a 9 de Setembro de 2008, IEEE Catalog Number CFP0890B-CDR, ISBN 978-1-4244-1736-0.

ELECTROMECHANICAL GOUGH--STEWART PLATFORM DIRECT DYNAMIC STUDY

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Publicado em:
Proceedings of the Controlo 2008 Conference– 8th Portuguese Conference on Automatic Control, Vila Real, 21 a 23 de Julho de 2008, pp. 200-2005.

Gough-Stewart platforms are variable length octahedral hexapods, with six degrees of freedom. They are usually used in the area of motion simulation and control. In the electromechanical Gough-Stewart platform referred in this paper the variable length legs are driven by electromechanical motors. The direct dynamic model of this electromechanical Gough-Stewart platform is presented. The model is implemented in simulation software and its results compared to the platform dynamics obtained using MSC.VisualNastran. The platform response to several leg movements' combination is also analyzed.

A FLYWHEEL ENERGY STORAGE SYSTEM WITH MATRIX CONVERTER CONTROLLED PERMANENT MAGNET SYNCHRONOUS MOTOR

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ABSTRACT

This paper presents an experimental characterization of a flywheel energy storage system. The device is based on steel seamless tube mounted as a vertical axis flywheel storing kinetic energy. The motor/generator is a Permanent Magnet Synchronous Machine controlled by an AC-AC Matrix Converter. The matrix control method uses a discrete-time model of the converter system to predict the future values of the input currents for all the 27 possible output voltage vectors generated by the matrix converter. An optimal controller minimizes current errors using a weighted cost functional. This flywheel and control process is intended for dynamic voltage restorer (DVR) to mitigate voltage sags.

Publicado em:
ICEM'08- XVIII International Conference on Electrical Machines, Vilamoura, Portugal, 6 a 9 de Setembro de 2008.

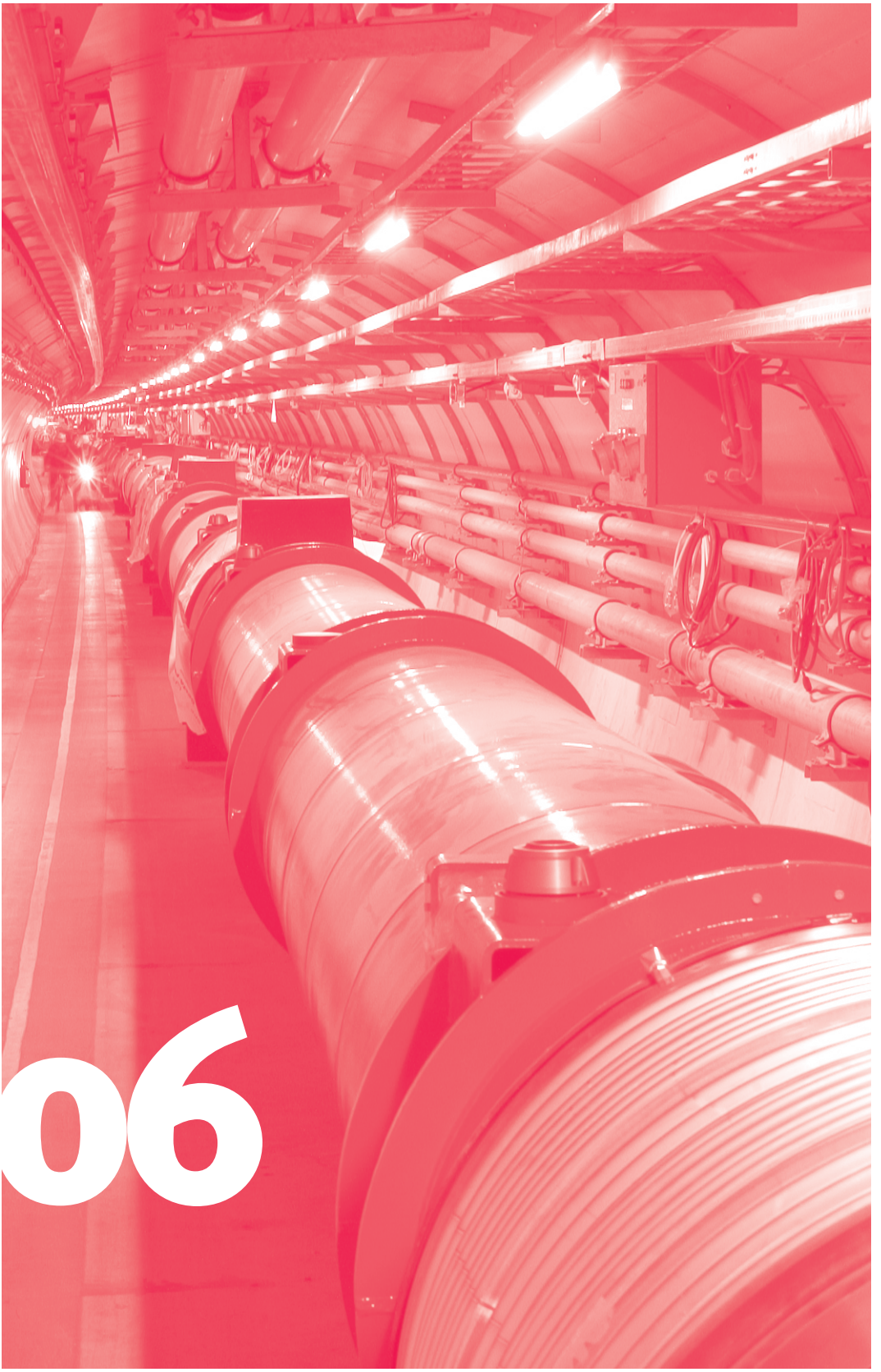
COMPORTAMENTO DE ACCIONAMENTOS ELECTROMECÂNICOS DE VELOCIDADE VARIÁVEL NUM BANCO DE ENSAIOS DE BOMBAS HIDRÁULICAS DO LNEC

Veiga Cardoso, Nuno Paulo Real da

Mestrado em: Engenharia Electrotécnica e de Computadores
Grau Concedido por: Universidade Técnica de Lisboa
Orientadores: Professor Doutor João Carlos Pires da Palma e Professor Doutor João José Esteves Santana
Provas Concluídas em: 26 de Novembro de 2008

Este trabalho pretende dar um contributo para o desenvolvimento de recursos para caracterização do comportamento de grupos de bombagem hidráulica no banco de ensaio de bombas do Laboratório de Ensaios Hidráulicos do Laboratório Nacional de Engenharia Civil. Nesta primeira fase, pretende-se avaliar o binário entregue pela máquina eléctrica à máquina hidráulica e, em alguns casos, o rendimento do próprio motor, uma máquina assíncrona trifásica de rotor em gaiola.
Existe uma dificuldade prática na medição de binário em grupos electrobomba por inserção de transdutores de binário, relacionada com a manobra de desacoplagem das duas máquinas, o que nem sempre é expedito ou sequer viável. Tal facto motivou a procura de métodos para observação indirecta do binário. A metodologia adoptada apela a uma modelação apropriada da máquina eléctrica e a medições efectuadas à custa dos ensaios clássicos da mesma.
Como as equações exactas para determinação dos parâmetros do esquema equivalente escolhido são não-lineares, a solução é obtida com recurso ao método iterativo de Newton-Raphson, procedimento de grande rapidez de convergência, adaptável a casos n-dimensionais. Os resultados de teste comprovam a validade da metodologia utilizada, por comparação com resultados obtidos através do Método F1 da norma IEEE Std 112-1996. A análise de sensibilidade permitiu concluir acerca da importância da qualidade da medição de cada grandeza necessária para obter o resultado final.

05



06

FÍSICA

Anuário Científico 2008

ISEL

BRANE ASSISTED QUINTESSENTIAL INFLATION WITH TRANSIENT ACCELERATION

Bento, M.C.[1]; González Felipe, R.[1,2]; Santos, N.M.C.[1]

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A simple model of quintessential inflation with the modified exponential potential $e^{-\alpha\phi}[A+(\phi-\phi_0)^2]$ is analyzed in the braneworld context. Considering re-heating via instant preheating, it is shown that the evolution of the scalar field ϕ from inflation to the present epoch is consistent with the observational constraints in a wide region of the parameter space. The model exhibits transient acceleration at late times for $0.96 \hat{} A\alpha^{2} \hat{} 1.26$ and $271 \hat{} \phi_0\alpha \hat{} 273$, while permanent acceleration is obtained for $2.3\times10^{-8} \hat{} A\alpha^{2} \hat{} 0.98$ and $255 \hat{} \phi_0\alpha \hat{} 273$. The steep parameter α is constrained to be in the range $5.3 \hat{} \alpha \hat{} 10.8$.

Publicado em:
Physical Review D, 2008, 77, 123512.

06

HELICAL TWISTING OF ELECTROSPUN CELLULOSE-BASED MICRO- AND NANOFIBERS

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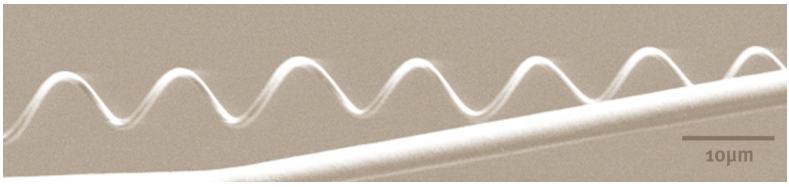
Publicado em:
Advanced Materials, 2008, 20, 4821-4825.

Helically twisted fibers can be produced by electrospinning liquid-crystalline cellulose solutions. Fiber topographies are studied by atomic force microscopy, scanning electron microscopy (see figure) and polarized optical microscopy. The fibers have a nearly universal pitch-to-diameter ratio and comprise both right- and left-handed helices.



EXPERIMENTAL RESULTS FOR THE RHEOLOGICAL AND RHEO-OPTICAL BEHAVIOR OF POLY(ETHYLENE TEREPHTHALATE)/LIQUID-CRYSTALLINE POLYMER BLENDS

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The use of thermoplastic/liquid-crystalline polymer (LCP) blends is recognized as a good strategy for reducing viscosity and improving mechanical properties relative to pure thermoplastics. This improvement, however, is only noticeable if the LCP fibrillates, in situ, during processing and the fibrils are kept in the solid state. In this article, we report a morphological, rheological, and rheooptics study performed with two blends of poly(ethylene terephthalate) with a LCP, Rodrun LC3000 (10 and 25 wt % LCP content), and we show that the obtained dropletshape relaxation time (the time the deformed droplet took to regain its spherical form after the cessation of flow) allowed for the explanation of the morphological observations. In fact, the droplet-shape relaxation time was higher for the blend with higher LCP content, for the higher experimentally accessible shear rates, and still increased at the highest shear rate, which explained the fibrils of the LCP dispersed phase observed in this blend, whereas for the lower LCP content blend, the droplet-shape relaxation time reached a low-value plateau for higher shear rates, which explained the absence of fibrillation in this blend.

Publicado em:
Journal of Applied Polymer Science, 2008, 107, 1280-1287.

06

HOW FOAM-LIKE IS THE SHEAR-INDUCED LAMELLAR PHASE OF AN IONIC LIQUID CRYSTAL?

Cruz, C.[1,2]; Godinho, M.H.[3]; Ferreira, A.J.[3]; Kulkarni, P.S.[4,5]; Afonso, C.A.M.[5]; Teixeira, P.I.C.[6,7]

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Publicado em:
Philosophical Magazine Letters, 2008, 88, 741-747.

In a recent article [M.H. Godinho et al., Liq. Cryst. **35**, 103 (2008)] we reported that sheared films of two n-alkylimidazolium salts exhibit liquid crystalline behaviour below their bulk equilibrium freezing temperature. The resulting morphologies are strongly reminiscent of two-dimensional liquid foams: the materials partition into dark domains (cells) separated by brighter (birefringent) walls, which are approximately arcs of circle and meet at vertices ("Plateau borders") with three or more sides. Here we investigate whether they satisfy known quantitative results for foams [see, *e.g.* D. Weaire and S. Hutzler, The Physics of Foams (Oxford University Press, Oxford, 1999)]. We find that: (i) where three walls meet, they do so at approximately 120 angles, for all times studied; (ii) Lewis's law of linear relation between cell area and number of sides is approximately satisfied at late times; (iii) the morphological patterns coarsen in time, both T1 and T2 processes are observed and, at late times, evolution is consistent with von Neumann's law; and (iv) relatively large numbers of 5-sided cells survive up to fairly late times. Results (i) and (iii) suggest that surface tension may play a key role in determining the physics of this system, as it does in low-viscosity liquid foams.

SHEAR-INDUCED LAMELLAR PHASE OF AN IONIC LIQUID CRYSTAL AT ROOM TEMPERATURE

Godinho, M.H.[1]; Cruz, C.[2,3]; Teixeira, P.I.C.[4,5]; Ferreira, A.J.[1]; Costa, C.[2,3]; Kulkarni, P.S.[6,7]; Afonso, C.A.M.[7]

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The phase behaviour of a number of N-alkylimidazolium salts was studied using polarizing optical microscopy, differential scanning calorimetry and X-ray diffraction. Two of these compounds exhibit lamellar mesophases at temperatures above 50uC. In these systems, the liquid crystalline behaviour may be induced at room temperature by shear. Sheared films of these materials, observed between crossed polarisers, have a morphology that is typical of (wet) liquid foams: they partition into dark domains separated by brighter (birefringent) walls, which are approximately arcs of circle and meet at "Plateau borders" with three or more sides. Where walls meet three at a time, they do so at approximately 120u angles. These patterns coarsen with time and both T1 and T2 processes have been observed, as in foams. The time evolution of domains is also consistent with von Neumann's law. We conjecture that the bright walls are regions of high concentration of defects produced by shear, and that the system is dominated by the interfacial tension between these walls and the uniform domains. The control of self-organized monodomains, as observed in these systems, is expected to play an important role in potential applications.

Publicado em:
Liquid Crystals, 2008, 35, 103-107.

06

GROWTH OF CUS PLATELET SINGLE CRYSTALS BY THE HIGH-TEMPERATURE SOLUTION GROWTH TECHNIQUE

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Publicado em:
Journal of Crystal Growth, 2008, 310, 2742–2745.

Millimeter size CuS single crystals with a dark indigo blue color and a plate hexagonal shape have been successfully grown by the high temperature solution growth technique using the KCl–LiCl eutectic as solvent. Surface microtopographic studies of the crystals indicated that the growth is made by the lateral spreading of the layers. Electrical resistivity measurements clearly show an anomaly at T~55 K, related with the low-temperature structural transition, a high residual resistivity ratio of ~400 and a sharp superconducting transition at T≈1.7 K confirming the very good quality of the crystals.

NATURAL INFLATION IN 5D WARPED BACKGROUNDS

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In light of the five-year data from the Wilkinson Microwave Anisotropy Probe (WMAP), we discuss models of inflation based on the pseudo Nambu-Goldstone potential predicted in five-dimensional gauge theories for different backgrounds: flat Minkowski, anti-de Sitter, and dilatonic spacetime. In this framework, the inflaton potential is naturally flat due to shift symmetries and the mass scales associated with it are related to 5D geometrical quantities.

Publicado em:
Physical Review D, 2008, 78, 023519.

06

MAGNETIZED STRANGE QUARK MATTER AND MAGNETIZED STRANGE QUARK STARS

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Publicado em:
Physical Review C, 2008, 77, 015807.

Strange quark matter could be found in the core of neutron stars or forming strange quark stars. As is well known, these astrophysical objects are endowed with strong magnetic fields that affect the microscopic properties of matter and modify the macroscopic properties of the system. In this article we study the role of a strong magnetic field in the thermodynamical properties of a magnetized degenerate strange quark gas, taking into account β-equilibrium and charge neutrality. Quarks and electrons interact with the magnetic field via their electric charges and anomalous magnetic moments. In contrast to the magnetic field value of 10^{19} G, obtained when anomalous magnetic moments are not taken into account, we find the upper bound $B^{\wedge}$ $8{,}6\times10^{17}$ G, for the stability of the system. A phase transition could be hidden for fields greater than this value.

DISCRETE AND CONTINUOUS SYMMETRIES IN MULTI-HIGGS-DOUBLET MODELS

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We consider the Higgs sector of multi-Higgs-doublet models in the presence of simple symmetries relating the various fields. We construct basis invariant observables which may in principle be used to detect these symmetries for any number of doublets. A categorization of the symmetries into classes is required, which we perform in detail for the case of two and three Higgs doublets.

Publicado em:
Physical Review D, 2008, 78, 116007.1-11607.10.

COMBINED EFFECTS OF STRONG AND ELECTROWEAK NEUTRAL CURRENT EFFECTIVE OPERATORS IN TOP QUARK PHYSICS AT THE CERN LHC

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Publicado em:
Physical Review D, 2008, 77, 114008.

Estudou-se os efeitos combinados dos operadores efectivos de dimensão seis na física das correntes neutras de mudança de sabor do quark top, passível de ser estudada no LHC, no CERN. Foram apresentadas diversas expressões analíticas para larguras de decaimento e secções eficazes de diversos processos de mudança de sabor, bem como uma análise da possibilidade da sua observação no LHC.

NOVA PORTARIA Nº 232/2008

Rodrigues, Carlos César

ACF - Dept. de Eng. Electrotécnica e Automação, ISEL, Lisboa, Portugal

O Regime Jurídico da Urbanização e da Edificação foi alterado pela Lei nº 60/2007, de 4 de Setembro, que remete a indicação dos elementos instrutores dos pedidos de realização de operações urbanísticas para portaria – a Portaria nº 232/2008, de 11 de Março.
A conformidade acústica das operações de loteamento, das obras de urbanização, edificação e demolição, bem como a autorização de utilização e a autorização de alteração de utilização, seja em fase de informação prévia, seja em fase licenciamento, seja em fase de comunicação prévia é, de acordo com a Portaria nº 232/2008, objecto de estudo e de verificação dos critérios estabelecidos na legislação aplicável em vigor.
A Portaria nº 232/2008 exige, também, quando aplicável, a apresentação de termos de responsabilidade subscritos pelo autor ou autores do respectivo Projecto Acústico, como garante do cumprimento das disposições legais e regulamentares aplicáveis.
A Portaria nº 232/2008 vem, desta forma, clarificar os pedidos de realização de operações urbanísticas, enunciando, num único diploma legal, todos os elementos que os devem instruir, nomeadamente os que às condições acústicas dizem respeito.

Publicado em:
Livro de Resumos do Seminário "Nova Legislação para Acústica de Edifícios", MRA Instrumentação, S.A., Faro, Funchal, Lisboa e Porto, Portugal, 2008.

SCORPIONATE COMPLEXES OF VANADIUM (III OR IV) AS CATALYST PRECURSORS FOR SOLVENT-FREE CYCLOHEXANE OXIDATION WITH DIOXYGEN

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Publicado em:
Pure Applied Chemistry, 2008, in press (doi:10.1351/PAC-CON-08-10-08).

The scorpionate vanadium complexes $[VCl_3\{HC(pz)_3\}]$ **1** (pz = pyrazolyl) and $[VCl_3\{SO_3C(pz)_3\}]$ **2** catalyze cyclohexane oxidation with dioxygen, to cyclohexanol (the main product) and cyclohexanone, under solvent-free conditions. Complex **1** provides the best activity (13% conversion into the ketone and alcohol, with high selectivity, at the O_2 pressure of 15 atm, at 140°C, 18 h reaction time). The reaction is further promoted (to 15% conversion) by pyrazinecarboxylic acid (PCA). The use of C- or O-radical traps supports the involvement of a free-radical reaction mechanism. The effects of various parameters were studied towards the optimization of the process.

A NEW CHEMICAL ROUTE TO SYNTHESISE TM-DOPED (TM = Co, Fe) TiO_2 NANOPARTICLES

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Since the discovery of ferromagnetism well above room temperature in the Co-doped TiO_2 system, diluted magnetic semiconductors based on TiO_2 doped with transition metals have generated great interest due to their potential use in the development of spintronic devices.
The purpose of this paper is to report on a new and swift chemical route to synthesise highly stable anatase single-phase Co- and Fe-doped TiO_2 nanoparticles, with dopant concentrations up to 10 at.% and grain sizes ranging between 20 and 30 nm. Complementary structural, microstructural and chemical analyses of the different nanopowders synthesised strongly support the hypothesis that a homogenous distribution of the dopant element in the substitutional sites of the anatase structure has been achieved. Moreover, UV-visible diffuse reflectance spectra of powder samples showed red shifts to longer wavelengths/lower energies and band gap energies decreasing with increasing Co or Fe concentration, which is consistent with n-type doping of the TiO_2 anatase matrix.
Films of Co-doped TiO_2 were successfully deposited onto Si (100) substrates via dip-coating method, using suspensions of $Ti_{1-x}Co_xO_2$ nanoparticles in ethylene glycol.

Publicado em:
European Journal of Inorganic Chemistry, 2008, 2008, 961-965.

06

KrF PULSED LASER ABLATION OF POLYIMIDE

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Publicado em:
Applied Physics A, 2008, 92, 957-961.

In the present paper, polyimide surfaces were processed with pulsed KrF laser radiation at fluences near the ablation threshold. The morphology of the processed surfaces was studied by scanning electron microscopy and chemical analyses performed by electron dispersive spectroscopy. The formation of conical structures was observed for radiation fluences lower than 0.5 J/cm^2. The areal density of cones increases with the number of pulses and decreases with the radiation fluence. At low fluences (‹150 mJ/cm^2), cones are formed due to shadowing by calcium phosphate impurities while for higher fluences the main mechanism of cones formation is believed to be radiation hardening.

MODIFICATION OF POLYIMIDE WETTABILITY BY KrF PULSED LASER ABLATION

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Laser ablation has been extensively studied in polymers because of their considerable utility in diverse fields such as medicine, microelectronics, photonics, etc. As a result, laser ablation of polymers has generated considerable interest in research during the past two decades. Among the many aspects of laser ablation of polymers, several authors have reported the formation and growth of conical structures during laser processing with UV laser radiation. Although this aspect of laser ablation has been investigated since the 1980s, only a few applications of these structures have been reported. In the present paper, we study the development of conical structures on polyimide treated with KrF laser radiation as a function of the radiation fluence, and its effect on the wettability of the polymer.

Publicado em:
Microscopy and Microanalysis, 2008, 14 S3, 73-76.

STRUCTURAL AND MICROANALYTICAL STUDIES OF CrO2 THIN FILMS ON c-SAPPHIRE BY HIGH RESOLUTION ELECTRON MICROSCOPY METHODS

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Publicado em:
Microscopy and Microanalysis, 2008, 14(S3), 47-48.

Chromium dioxide (CrO_2) has been extensively used in the magnetic recording industry. However, it is its ferromagnetic half-metallic nature that has more recently attracted much attention, primarily for the development of spintronic devices. CrO_2 is the only stoichiometric binary oxide theoretically predicted to be fully spin polarized at the Fermi level. It presents a Curie temperature of ~ 396 K, *i.e.* well above room temperature, and a magnetic moment of 2 μ_B per formula unit. However an antiferromagnetic native insulating layer of Cr_2O_3 is always present on the CrO_2 surface which enhances the CrO_2 magnetoresistance and might be used as a barrier in magnetic tunnel junctions.

Here we report on high resolution electron microscopy structural and analytical studies of CrO_2 films deposited onto Al_2O_3 (0001) by atmospheric pressure CVD from CrO_3 precursor. As reported previously films were grown within a broad range of deposition temperatures from 320 to 410°C, and oxygen carrier gas flow rates of 50 – 500 sccm. Herein we will show the results obtained for two films grown at 340 and 360°C with 100 sccm oxygen.

Cross-sectional specimens for TEM were prepared by mechanical grinding, dimpling and argon ion-milling of the samples in a liquid-nitrogen-cooled holder with an acceleration voltage of 5 keV and an incidence angle of 8°. Analytical TEM and HREM studies were carried out using a Philips Tecnai 20F FEG microscope operating at 200 keV, equipped with an Energy Dispersive X-Ray (EDX) analysis system and a scanning transmission electron microscopy modulus (STEM) with a high angle annular detector (HAAD) for Z-contrast imaging and composition mapping. Electron diffraction pattern (EDP) and simulations using Fast Fourier transform (FFT) of the HREM images were used to analyze the crystal structure.

WETTING TRANSITION OF A NEMATIC LIQUID CRYSTAL ON A PERIODIC WEDGE-STRUCTURED SUBSTRATE

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It is known that the wetting behaviour of a fluid is deeply altered by the presence of rough or structured substrates. We first review some simple considerations about isotropic fluids and rough substrates, and then we generalize Wenzel's law, which assigns an effective contact angle to a droplet on a rough substrate, when the wetting layer has an ordered phase, like a nematic. We estimate the conditions for which the wetting behavior of an ordered fluid can be qualitatively different from that usually found in a simple fluid. To support our general considerations, we use the Landau-de Gennes mean field approach to investigate theoretically and numerically the wetting transition of a nematic phase on a periodic triangular structured substrate.

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Eur. Phys. J. E, 2008, 26, 97-101.

MAGNETIC PROPERTIES OF Co-DOPED TiO_2 ANATASE NANOPOWDERS

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Publicado em:
Applied Physics Letters, 2008, 93, 222502-222504.

This letter reports on the magnetic properties of $Ti_{1-x}Co_xO_2$ anatase phase nanopowders with different Co contents. It is shown that oxygen vacancies play an important role in promoting long-range ferromagnetic order in the material studied in addition to the transition-metal doping. Furthermore, the results allow ruling out the premise of a strict connection between Co clustering and the ferromagnetism observed in the Co:TiO_2 anatase system.

SURPRISES OF THE TRANSFORMER AS A COUPLED OSCILLATOR SYSTEM

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We study a system of two RLC oscillators coupled through a variable mutual inductance. The system is interesting because it exhibits some peculiar features of coupled oscillators: (i) there are two natural frequencies; (ii) in general, the resonant frequencies do not coincide with the natural frequencies; (iii) the resonant frequencies of both oscillators differ; (iv) for certain choices of parameters, there is only one resonant frequency, instead of the two expected.

Publicado em:
European Journal of Physics, 2008, 29, 413-420.

HALF-SANDWICH SCORPIONATE VANADIUM, IRON AND COPPER COMPLEXES: SYNTHESIS AND APPLICATION IN THE CATALYTIC PEROXIDATIVE OXIDATION OF CYCLOHEXANE UNDER MILD CONDITIONS

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Publicado em:
Advanced Synthesis and Catalysis, 2008, 350, 706-716.

The new half-sandwich scorpionate complexes $[VCl_3\{HC(pz)_3\}]$ **1** (pz = pyrazolyl), $[VCl_3\{SO_3C(pz)_3\}]$ **2**, $[FeCl_2\{HC(pz)_3\}]$ **3**, $Li[FeCl_2\{SO_3C(pz)_3\}]$ **4** and $[CuCl\{SO_3C(pz)_3\}]$ **5** were synthesized, characterized and shown to act, as well as the related $[CuCl_2\{HC(pz)_3\}]$ **6**, as selective catalysts (or catalyst precursors) for the peroxidative oxidation (by H_2O_2) of cyclohexane to cyclohexanol and cyclohexanone, under mild conditions (at room temperature and using an aqueous solution of H_2O_2). The iron complexes are the most active ones (reaching TON values up to *ca.* 690), the effects of a variety of factors are reported and the reaction is shown to proceed via both C- and O-centred radical mechanisms, conceivably involving a metal-based oxidant.

INTERACTIONS BETWEEN CIRCULAR INCLUSIONS IN SMECTIC-C FILMS WITH PLANAR ANCHORING

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We investigate analytically the interaction between circular inclusions in smectic-C films with planar anchoring. We present a rigorous solution for an isolated circular colloid with planar anchoring and use it to calculate the interaction between two circular colloids, approximately. At large separations the interaction is quadrupolar and we show that at short range two different regimes may be observed. For weak anchoring, the interaction is always attractive in some directions, which may lead to particle contact or coalescence. However, for strong anchoring, the interaction exhibits a well defined minimum, for colloids at a particular separation and given relative orientation. The equilibrium configuration was found to depend on the anchoring strength.

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Mol. Cryst. Liq. Cryst., 2008, 495, 266-273.

KrF EXCIMER LASER ABLATION OF HUMAN ENAMEL

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Publicado em:
Materials Science Forum, 2008, 587-588, 42-46.

Laser treatment is a promising technique for dental applications such as caries prevention, dental hypersensitivity reduction and improvement of bond strength of restoration materials. In this study the morphological. structural and chemical changes of enamel surface due to treatment with KrF excimer laser radiation were evaluated using scanning electron microscopy. X-ray diffraction, and X-ray photoelectron spectroscopy. For radiation fluences near 1 J/cm^2, laser processing originates a relatively porous surface due to preferential removal of material in the enamel prism sheaths. Increasing the fluence leads to a relatively flat surface with clear evidence of surface melting. The X-ray diffractograms of both treated and untreated enamel are similar and correspond to hydroxyapatite. The only modification due to the laser treatment is a slight shift of the peaks, probably. due to a loss of the structural water of hydroxyapatite. X-ray photoelectron spectroscopy confirmed that organic matter is removed from the irradiated surface but no significant changes in the mineral phase occur.

COHERENCE THRESHOLDS IN MODELS OF LANGUAGE CHANGE AND EVOLUTION: THE EFFECTS OF NOISE, DYNAMICS AND NETWORK OF INTERACTIONS

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A simple model of language evolution proposed by Komarova, Niyogi, and Nowak is characterized by a payoff in communicative function and by an error in learning that measure the accuracy in language acquisition. The time scale for language change is generational, and the model's equations in the mean-field approximation are a particular case of the replicator-mutator equations of evolutionary dynamics. In well-mixed populations, this model exhibits a critical coherence threshold; *i.e.*, a minimal accuracy in the learning process is required to maintain linguistic coherence. In this work, we analyze in detail the effects of different fitness-based dynamics driving linguistic coherence and of the network of interactions on the nature of the coherence threshold by performing numerical simulations and theoretical analyses of three different models of language change in finite populations with two types of structure: fully connected networks and regular random graphs. We find that although the threshold of the original replicator-mutator evolutionary model is robust with respect to the structure of the network of contacts, the coherence threshold of related fitness-driven models may be strongly affected by this feature.

Publicado em:
Physical Review E, 2008, 77, 046108.

06

EFFECT OF SALT-MARSH PLANTS ON THE MOBILITY OF CR IN SEDIMENTS

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Publicado em:
Ciencias Marinas, 2008, 34(3), 363–372.

Depth variation (1-cm resolution) of total Fe, Mn, and Cr concentrations was determined in below-ground biomass of *Halimione portulacoides* and in root sediments from two Tagus Estuary salt marshes (Portugal). The metal fractions extracted by hydroxylamine (HYD) and HCl were also quantified in sediment samples. Edaphic conditions of the sediment (O_2, pH, E_H, acid-volatile sulphides [AVS], and root biomass) were characterized in both marshes. Higher dissolved oxygen concentrations were found at depths with increased root biomass, while AVS were nearly absent in the root zone increasing with depth. Sediments colonized by *H. portulacoides* showed higher variability of total metal concentrations with depth than non-vegetated sediments, possibly due to intense exchanges between the below-ground plants and surrounding sediments. Concentrations of Fe_{HYD} (mainly Fe oxyhydroxides) were elevated in the root sediments since Fe(II) is oxidized by the O_2 released from roots. The normalization of Cr_{HYD} levels to Fe_{HYD} showed a sharp increase when oxygen is depleted, suggesting that Cr is sequestered in the Fe oxyhydroxide fraction. Roots of *H. portulacoides* from both marshes showed little 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. The inability or limited defence mechanisms of *H. portulacoides* to accumulate Cr indicates that this halophyte is not adequate for successfully phytostabilizing Cr-polluted marshes.

CHARACTERIZATION OF THE SEISMIC ANISOTROPY AND DISCONTINUITIES IN THE IBERIAN AND SOUTHWEST MARGIN - PRELIMINARY RESULTS

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Seismic anisotropy is the variation of the properties of seismic waves propagation, as result of the presence of preferential alignments of micro-cracks or other heterogeneities in the crust, or olivine crystals in the mantle. The origin of crustal anisotropy is related with the state of local and/or regional tension, whereas mantle anisotropy is a product of induced deformation in the astenosphere by recent or preserved past movements. The goal of this work is a study of deep structure and anisotropy of the crust and mantle beneath part of the Iberian Peninsula and neighbouring regions. The lithosphere of the Iberian Peninsula and its margins has suffered a number of processes of collision and extension. In the Lower Paleozoic, the collision of three tectonics blocks produced the Variscan Orogeny, the main event of formation of the Iberia lithosphere. The south interaction between Africa and Iberia is characterized, since the Miocene, for a diffuse convergent margin that originates a vast area of deformation. The impact of this complex tectonic structure of the lithosphere remains an incognito.

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Actas da 6º Assembleia Luso-Espanhola de Geodesia e Geofísica, Tomar, 11 a 14 de Fevereiro de 2008, pp..

EXPERIMENTAL RESULTS ON ELECTRORHEOLOGY OF LIQUID CRYSTALLINE POLYMER SOLUTIONS

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Actas do XVth International Congress on Rheology, Monterey - California, 3 a 8 de Agosto de 2008, pp. 1429-1431.

The electrorheological (ER) effect is known as the enhancement of the apparent viscosity upon application of an external electric field[1].
Suspensions of polarizable particles in non-conducting solvents are the most studied electrorheological fluids, however, liquid crystalline materials may also present ER effect as long as their dielectric anisotropy is positive[2,3]. In the liquid crystalline state of a positive dielectric anisotropy, the application of the electric field makes the director align perpendicular to the flow direction, thus increasing the apparent viscosity.
In this work results of two liquid crystalline polymer solutions, acetoxypropylcellulose (APC) in dimethylacetamide (DMAc) and poly- -benzyl-L-glutamate (PBLG) in 1,4-dioxane, presenting opposite behavior upon application of the electric field, will be presented. APC/DMAc (negative dielectric anisotropy) presents a decrease of the apparent viscosity upon application of the electric field, as expected, while PBLG/1,4-dioxane (positive dielectric anisotropy) presents the opposite behavior. For this last solution we will present the shear flow curves for different electric fields in function of polymer molecular weight and solution concentration.

SURFACE MODIFICATION OF DENTAL HARD TISSUES USING PULSED UV LASERS

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In the present paper the main results achieved by the authors in the study of laser ablation and surface texturing of dentin and enamel with KrF excimer laser radiation will be reviewed. In dentin, the laser treatment leads to two distinct behaviors. When the tubules are roughly parallel to the laser beam, a coneshaped topography develops for fluences between 0.5 and 2 J/cm^2. When the tubules are significantly tilted towards the laser beam or/and the fluence exceeds 2 J/cm^2, the treated surface is flat and covered with resolidified material. The kinetics of cone growth can be described by a modified Johnson-Mehl-Avrami-Kolmogorov equation and the boundary lines delimiting fully developed cones define a Voronoi tessellation. In enamel, material is preferentially removed at the prisms sheaths leading to the formation of surface pits of a few micrometers. The laser treatment leads to a reduction of the organic matter content of dental hard tissues, without significantly affecting hydroxyapatite.

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Actas da 3rd Pacific International Conference on Application of Lasers and Optics (PICALO 2008), Laser Institute of America, Beijing, China, 16 a 18 Abril 2008, p. 82. 2008.

HALL TRANSPORT MEASUREMENTS IN CVD GROWN CrO_2 FILMS ON Al_2O_3 (0001)

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Publicado em:
Livros de Resumos da Joint European Magnetics Symposia - JEMS'08, Dublin, Irlanda, 14 a 19 de Setembro de 2008.

Of the numerous ferromagnetic materials predicted to be half-metallic (having a transport spin polarization, P=100%) only CrO_2 has been found to be close to this idealised behaviour in point contact Andreev reflection spectroscopy (PCAR) experiments. CrO_2 also has a relatively high Curie temperature of ~400K and this combination of properties makes CrO_2 a very attractive material for spintronic applications. However, the resistivity of CrO_2 has an unusual and strong temperature dependence between base and room temperature indicating a change in transport mechanism in this temperature range. Here we study resistance, Hall and PCAR spectroscopy of CVD CrO_2 films with a range of thicknesses and grain sizes. We find that the residual resistivity ratio in the films is governed by carrier mobility not carrier density, that the carriers are holes and that the hole mobility is correlated with grain size. Anomalous Hall measurements have been used to investigate the temperature dependence of the spin polarization in other materials systems. We find that in CrO_2 it is the mobility (scattering time) that is the dominant factor in the anomalous Hall conductivity, but that it is possible to probe the temperature dependence of the transport spin polarization by synthesizing films in the dirty limit with short scattering times at all temperatures. In this regime the anomalous Hall conductivity and hence the transport spin polarization is nearly temperature independent up to room temperature. We have previously observed temperature independent spin polarization in the dirty metal regime in the Heusler alloy Co_2MnSi.

STRAIN AND INTERFACE EFFECTS ON THE MAGNETIC AND TRANSPORTPROPERTIES OF $LA_{0.7}CA_{0.3}MNO_3$/CAO MULTILAYERS

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$La_{0.7}Ca_{0.3}MnO_3$/CaO (LCMO/CaO) multilayers were deposited on (100) $LaAlO_3$ substrates by pulsed injection metal organic chemical vapour deposition. The samples were characterised by X-ray diffraction, transport and magnetization measurements. An anomalous behaviour of the electrical resistance under applied magnetic field and an exchange bias effect for the magnetization are observed for the multilayers with thinner LCMO layers. These results suggest the existence of a short range antiferromagnetic coupling at the layer interfaces.

Publicado em:
Livro de Resumos da International Conference on Superconductivity and Magnetism, Side, Turquia, 26 a 29 Agosto de 2008.

WAVEFORM SIMILARITY AND HYPOCENTRAL RELOCATION OF THE JULY 1998 FAIAL SEISMIC SWARM

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Livros de Resumos da 6ª Assembleia Luso-Espanhola de Geodesia e Geofísica, Tomar, 11 a 14 de Fevereiro de 2008.

An aftershocks sequence usually possesses highly similar waveforms due to similar focal mechanisms and propagation paths. The procedure to identify similar waveforms within a seismic records dataset is based on waveform cross-correlation and a clustering method; it allows a precise relocation of the events and the determination of the common focal mechanism, thus improving the outline of the tectonic structures. For the aftershock sequence triggered by the 9th July 1998 Faial earthquake, we obtained a dataset of 525 hypocenters divided into several clusters of similar events. The relocation of the largest clusters, together with the their composite focal mechanisms, partially confirmed some of the results previously obtained, with clusters oriented along one of the main tectonic direction of the Azores plateau, N150E. However, the results also point to a revaluation of the importance of the other dominant tectonic direction, N120E, more relevant in seismogenic terms than previously assumed.

FOAM-LIKE BEHAVIOUR OF LAMELLAR IONIC LIQUID CRYSTALS

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N-alkylimidazolium salts have been shown to order into either columnar and lamellar mesophases. This liquid crystalline behaviour can be induced at room temperature by shear. Sheared films of the lamellar phase of these compounds observed between crossed polars exhibit a morphology that is typical of (wet) liquid foams: they divide into dark domains separated by brighter (birefringent) walls which are approximately arcs of circle and meet in “Plateau borders” with three or more sides. Where walls meet three at a time, they do so at approximately 120° angles. These patterns coarsen with time, both T1 and T2 processes having been observed, as in foams. The time evolution of domains is also consistent with von Neumann's law: domains with fewer than 6 sides shrink and disappear, whereas those with 6 or more sides either remain unchanged or increase in area. We conjecture that the bright walls are regions of high concentration of defects produced by shear, and that the system is dominated by the interfacial tension between these walls and the uniform domains.

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Livro de Resumos da 7th Liquid Matter Conference, Lund, Suécia, Junho/Julho 2008.

06

HOW FOAM-LIKE IS THE SHEAR-INDUCED BEHAVIOUR OF LAMELLAR IONIC LIQUID CRYSTALS?

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Publicado em:
Livro de Resumos da 22nd International Liquid Crystal Conference, Jeju, Coreia, Junho/Julho 2008.

In a recent paper we reported that sheared films of two n-alkylimidazolium salts exhibit liquid crystalline behaviour below their bulk equilibrium freezing temperature. The resulting morphologies are strongly reminiscent of two-dimensional liquid foams: the materials partition into dark domains (cells) separated by brighter (birefringent) walls, which are approximately arcs of circle and meet at vertices ("Plateau borders") with three or more sides. Here we investigate whether they satisfy known quantitative results for foams[2]. We find that: (i) where three walls meet, they do so at approximately 120° angles, for all times studied; (ii) Lewis's law of linear relation between cell area and number of sides is approximately satisfied at late times; (iii) the morphological patterns coarsen in time, both T1 (neighbour switching) and T2 (cell disappearance) processes are observed and, at late times, evolution is consistent with von Neumann's law; and (iv) relatively large numbers of 5-sided cells survive up to fairly late times. Results (i) and (iii) suggest that surface tension may play a key role in determining the physics of this system, as it does in low-viscosity liquid foams.

HOW FOAM-LIKE IS THE SHEAR-INDUCED BEHAVIOUR OF LAMELLAR IONIC LIQUID CRYSTALS?

Ferreira, A.J.[1]; Godinho, M.H.[1]; Cruz, C.[2,3]; Kulkarni, P.S.[4,5]; Afonso, C.A.M.[5]; Teixeira, P.I.C.[6,7]

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In a recent paper we reported that sheared films of two n-alkylimidazolium salts exhibit liquid crystalline behaviour below their bulk equilibrium freezing temperature. The resulting morphologies are strongly reminiscent of two-dimensional liquid foams: the materials partition into dark domains (cells) separated by brighter (birefringent) walls, which are approximately arcs of circle and meet at vertices ("Plateau borders") with three or more sides. Here we investigate whether they satisfy known quantitative results for foams. We find that: (i) where three walls meet, they do so at approximately 120° angles, for all times studied; (ii) Lewis's law of linear relation between cell area and number of sides is approximately satisfied at late times; (iii) the morphological patterns coarsen in time, both T1 (neighbour switching) and T2 (cell disappearance) processes are observed and, at late times, evolution is consistent with von Neumann's law; and (iv) relatively large numbers of 5-sided cells survive up to fairly late times. Results (i) and (iii) suggest that surface tension may play a key role in determining the physics of this system, as it does in low-viscosity liquid foams.

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LIQUID CRYSTALLINE SPINNING OF CELLULOSE NANOFIBERS

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Publicado em:
Livro de Resumos da Advanced Nanomaterials 2008, Aveiro, Portugal, Junho 2008.

The material from which silk is spun is liquid crystalline, spiders can draw it during extrusion into a hardened fibre using minimal forces. Spider silk has exceptional mechanical properties though it is spun at close to ambient temperatures and pressures using water as the solvent. Cellulose is a naturally occurring polymer of particular interest due to its abundant accessibility and biodegradability. These properties make cellulose fibers useful in a wide range of areas, such as filtration, biomedical applications, and protective clothing. Cellulose and cellulose derivatives can also generate liquid crystalline phases and the fibers produced from those phases are expected to have enhanced mechanical properties like spider's silk. In the literature, a large variety of polymers have been successfully electrospun into fibers. However, the electrospinning characteristics of liquid crystalline solutions from cellulose derivatives have not been investigated as far as we are aware. The application of electrospun nanofibers from cellulose liquid crystalline solutions has never been investigated. In this work we prepared nanofibers by electrospinning from cellulose liquid crystalline solutions. Scanning electron microscope (SEM), atomic force microscopy (AFM) and polarising optical microscopy (POM) give evidence of the formation of a non-woven mat of submicron-sized cellulose fibers (250-750 nm in diameter). We have nvestigated systematically the electrospinning characteristics of the lyotropic cellulose solution; results have been analyzed in the context of a microscopic model for the tertiary structure of a chiral, helix-forming polymer in an external electric field.

MICRO- AND NANOSTRUCTURES FROM LIQUID CRYSTALLINE CELLULOSE MATERIALS

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Cellulose and cellulose derivatives can form cholesteric liquid crystalline (LC) phases in a wide variety of organic solvents. In addition to these lyotropic solutions, a series of esters of hydroxypropylcellulose have been found to exhibit thermotropic cholesteric phases at room temperature.

Tunable topographical films were prepared from lyotropic cellulose systems. Atomic force microscopy (AFM) measurements indicate that the features on the film surfaces can be manipulated by controlling the processing conditions, and a fractal analysis of these surfaces indicates a scale-invariant nature between 300 nm and 4 μm. Recently it was found that helical micro and nano springs can be obtained from cellulose liquid crystalline phases by the electrospinning technique (figure). In fact, cellulose acetate was the first fiber reported to have been electrospun and is the most popular cellulosic material for electrospinning today. The diameter of the fibers can be significantly reduced from micrometers to a few nanometers using this technique.

In this work we report the observation of micro and nano structures obtained from cellulose liquid crystalline systems, namely helical twisting in electrospun cellulosic fibres. The twisting is on a supramolecular scale, and similar to what has been seen in other systems such as amyloid (polypeptide) nanofibrils and cellulose from micrasterias denticulate. Three different imaging techniques have been employed to quantify this: atomic force microscopy (AFM), scanning electron microscopy (SEM) and polarized optical microscopy (POM). Future applications of these systems will be discussed.

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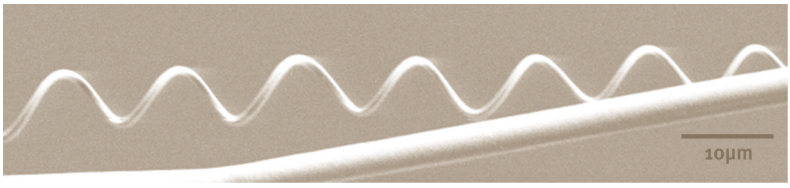

Figure 1. Scanning electron microscopy (SEM) image of a helix obtained from a cellulose based liquid crystalline material by electrospinning.

MECHANICAL CHARACTERIZATION OF BRITTLE MATERIALS – TOMOGRAPHY OF SMALL BODIES BY ULTRASONIC TRAVEL-TIME TOMOGRAPHY

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1. INTRODUÇÃO

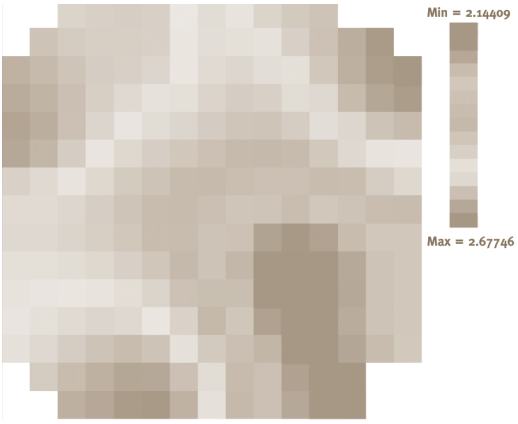
O Laboratório de Monitorização Microsísmica da Área Científica de Física do Instituto Superior de Engenharia de Lisboa, adquiriu recentemente equipamento para investigação nos domínios dos ultrasons, e da emissão acústica.

O equipamento é constituído por um sistema de aquisição "ESG – Hyperion GIGA Recorder" de 8 canais com uma taxa de amostragem de 10 MHz e uma dinâmica de 16 bit. O sistema é controlado por uma "work station" Dell OptiPlex de 2,8 GHz através de um software ESG - Hypacq. O laboratório possui actualmente 2 tipos de sensores piezocerâmicos: 4 transductores para uma gama de frequências de 0,02 MHz a 0,20 MHz e 8 transductores para uma gama de frequências de 0,15Mhz a 0,70 MHz. O sistema é completado com diverso equipamento entre o qual se destacam 8 pré amplificadores "Physical Accoustic Corporation" de duplo ganho (40 dB – 60 dB), um sistema de controle dos sensores e pulsador – "trigger" para selecção de emissão-recepcção - e um conversor analógico digital. O software de processamento do sinal inclui módulos de localização automática de eventos, visualização 2D e 3D, de ondas e software de tomografia.

2. TOMOGRAFIA SÍSMICA

Os primeiros estudos desenvolveram-se sobre um modelo em acrílico "perspex" constituído por uma placa quadrada de 13cm de lado e 2cm de espessura, no qual foi realizado um furo circular, descentrado. Nesta experiência foi utilizado uma rede de 8 sensores/receptores, que foram sendo sucessivamente deslocados ao longo das arestas da placa.

Em cada experiência, um dos sensores funcionou como emissor e os restantes oito como receptores. O sinal final em cada sensor é o resultado do "stacking" de 100 impulsos emitidos pelo emissor. A geometria desta rede foi sucessivamente mudada, de forma a obter uma boa distribuição azimutal dos trajectos emissor-receptor. Pretendia-se obter: (1) a caracterização da anisotropia azimutal das velocidades de



propagação da ondas volúmicas e (2) a possibilidade de por meio de inversão localizar a zona "vazia" da placa de perspex.
A obtenção de 66 trajectos permitiu determinar variações azimutais na velocidade de propagação de ondas volúmicas (2,52 mm/µs a 2,65 mm/µs) e, por inversão através de um algoritmo SIRT - Simultaneous Iterative Reconstruction Technique, Iyer, H. e Hirahara (1993), foi possível localizer a descontinuidade de velocidades (v ‹ 2,2 mm/µs) associada ao vazio (furo circular na placa).

3. CORRELAÇÃO ENTRE A ANISOTROPIA SÍSMICA, ANISOTROPIA MAGNÉTICA E ORIENTAÇÃO PREFERENCIAL DE FABRIC EM ROCHAS MAGMÁTICAS

Está em curso um estudo de comparação laboratorial entre as velocidades de propagação ultrasónicas, anisotropia de susceptibilidade magnética e da orientação preferencial do fabric petrográfico sobre uma amostra de um basanito ultramáfico da soleira da Foz da Fonte (Espichel). Os estudos magnéticos e de fabric previamente realizados sobre esta rocha, Miranda, R. *et al.* (2006), permitiram conhecer a orientação do elipsóide de susceptibilidade magnética e a sua relação com a orientação preferencial das plagioclases e dos minerais opacos, essencialmente óxidos de Fe e Ti.
Numa primeira fase deste estudo está-se a proceder a determinações das velocidades ultrasónicas de forma a caracterizar a anisotropia azimutal, em três planos ortogonais. Estas medidas são feitas à pressão e temperatura ambiente.

MAGNETIC AND PALEOMAGNETIC INVESTIGATIONS IN THE FOZ DA FONTE SILL

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Livros de Resumos do 6ª Assembleia Luso-Espanhola de Geodesia e Geofísica, Tomar, 2008.

The Foz da Fonte sill outcrops at a N-S coastal section in the Setúbal peninsula, south of Lisbon. Its top is exposed over an area of approximately 300m^2. It is about 8m thick inducing a metamorphic aureole in the Lower Cretaceous sedimentary country rock of Aptian age, Kullberg (2000).

The sill is made up by fine grained ultramafic (SiO_2<45%) alkaline basanites. containing Ti-augite, kaersutite, plagioclase, apatite, opaque minerals and late carbonates that fill vesicles and fractures. Its alkaline nature places it in the third and last cycle of mesozoic magmatic activity Portuguese territory (100-70 Ma - Martins, 1991) that includes the subvolcanic massifs of Sintra, Sines and Monchique, the Lisbon volcanic complex and other minor intrusives.

Important positive magnetic anomalies onshore and offshore the West Iberian Margin define linear trends from the Tore seamount to the Guadalquivir bank, encompassing the three subvolcanic alkaline massifs (Sintra Sines and Monchique) and a large magnetic anomaly just West of the studied sill , Silva *et al* (2000).

The main objectives of this work are:

1. Find the direction, and if possible the sense, of the magmatic flow during the emplacement of the sill.; therefore we attempt to infer the style of magma feeding system: linear (pipe) or planar (dyke or fissural) feeder.
2. Understand the relationship of this intrusion with the large magnetic anomaly, of probable magmatic origin, offshore, west of the study area.
3. magnetic and paleomagnetic characterization of the structure.

We used the anisotropy of magnetic susceptibility (AMS) to characterize the magnetic fabric and to deduce the magmatic flow pattern For this study samples were collected from 19 stations throughout the sill's top. At least 5 specimens per station were obtained, totalling 109 specimens that were analysed for the determination of their AMS fabrics using a Kappabridge KLY-2. The average magnetic susceptibility is **k** = 74 ± 17 (10^{-3} SI) and the average shape of the ellipsoid of susceptibility is prolate with magnetic lineation **L** = 1,022 ± 0,002 and

magnetic foliation **F** = 1,015 ± 0,008. The average degree of magnetic anisotropy is low, **P** = 1,038 ± 0,015.
The magnetic fabric is triaxial, everywhere and the measured magnetic properties (bulk and anisotropy susceptibilities) are very consistent and steady across the sill.
Thermomagnetic analysis under argon atmosphere shows one main magnetic phase with Curie temperature of 570° ± 14° and traces of a minor phase with Curie temperature below 3500°C.
In the majority of the stations the magnetic lineation has a general WNW-ESE orientation (figure 1). The average magnetic lineation is extremely well defined with K_1 = 118°/1° (azimuth/inclination) and a very small ellipse of confidence with semi-axes e_{13} = 1.3° and e_{21} = 3.0°.
The magnetic foliation plane is also very well defined and with the exception of one station, it is sub-horizontal everywhere but slightly imbricated relative to the sill top. Average values for K_3 axis, are 204°/84° and the semi-axes of the confidence ellipse are e_{13} = 1,3° and e_{23} = 3.1° (figure 1).
Paleomagnetic data exhibit variations in demagnetization behavior but 12 samples gave consistent results. Most of these samples show, in a orthogonal projection, a linear progression of the declination and inclination to the origin (Fig. 2). By 20 mT, the initial magnetization is usually already reduced to 25%. After orientation correction due to the structural tilt of the sil, (based on the orientation of the enclosed sedimentary rock) this group defines a NRM direction D_m= 329,1, I_m = 32,0 and α_{95} = 5,9 and a VGP 56N, 231E.

INTEGRATED FABRIC ANALYSIS (MAGNETIC AND PETROGRAPHIC) FOR MAGMA FLOW DETERMINATION OF THE MAFRA RADIAL DYKE SWARM (PORTUGAL)

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Livro de Resumos Geophysical Research Abstracts, Vol. 10, EGU2008-A-10708, 2008, SRef-ID: 1607-7962/gra/EGU2008-A-10708, EGU General Assembly 2008.

The anisotropy of magnetic susceptibility (AMS) has been considered a reliable tool for characterization of petrofabrics of rocks from a wide range of geological settings for at least the last four decades, with particular use for magma flow studies on dykes when the petrofabric is not evident. However, the assumption that the magnetic lineation (K1) should be considered as the inferred magma flow direction when in presence of normal magnetic fabrics is still controversial in face of discrepancies to flowrelated magmatic petrofabrics described on several other studies. Recent fabric analysis integrating AMS together with magma flow-related petrofabrics (SPO of plagioclases and deformed vesicles) on shallow dykes from the Mafra Radial Dyke Swarm (MRDS) proved to be a check-test to the usually adopted AMS criteria.

The MRDS is assigned to the Late Cretaceous alkaline cycle of the western Iberia continental margin associated with the opening of the North Atlantic, but still poorly understood. Its radial pattern, unique in the Lusitanian Basin, suggests that at the time of emplacement the deviatoric stress should have been very low, which is in agreement with an emplacement after the rift phases and before the tectonic inversion. The petrofabrics (micro and mesoscale) were investigated independently and then compared with the magnetic fabric, and in special, with the magnetic lineation direction. First, the SPO analysis of plagioclase micro-phenocrystals and the opaque minerals were processed accordingly to the Intercepts method on oriented thin sections cut within the magnetic planes K1K2 (magnetic foliation plane) and K1K3 (perpendicular to the dyke margins) to confirm that the petrofabric was flow-related. Second, the presence of oriented elongated vesicles in the dykes was used to perform an analysis of magma flow within the dyke and estimate a mean flow direction. Sampling was carried out on the margins of narrow vertical basalt/dolerite dykes, trending WNW-ESE, where the flow-related fabrics are expected to be more expressive.

Approximately 200 standard sized oriented samples were collected. The magnetic susceptibility measurements were made using a

Kappabridge KLY-2 (Agico, Brno) susceptibility bridge and the principal magnetic phases were examined by thermo-magnetic analysis in low magnetic field using a CS23 (Agico, Brno) furnace apparatus coupled to the KLY-2 susceptibilimeter, in an argon-controlled environment, up to a temperature of 700°C. The AMS ellipsoid is defined by a second-order tensor. Statistical treatment of directional data was made using the bivariate extension of Fisher's statistics determining the uncertainties of each principal susceptibility direction for all samples and establishing 95% confidence ellipses for each mean principal susceptibility directions.
The bulk susceptibility (K) show a bimodal distribution (values from 0.2-600x10—3 SI), showing clearly the existence of low and high susceptibility dykes. The main magnetic carriers are titanomagnetites with different oxidation levels. The dominant AMS ellipsoid shape is oblate for both shape parameters, T and L — F, indicating a major importance of the magnetic planar fabric over the linear fabric. The magnetic fabric of all dykes show good clustering of minimum susceptibility axis (K3) close to the dyke pole and generally good clustering of the maximum (K1) and intermediate (K2) axis, with small non-overlapping confidence ellipses (K3 confidence ellipses smaller than K1 confidence ellipses), establishing a tri-axial magnetic fabric with a well defined magnetic foliation plane (MFP). This corresponds to typical normal magnetic fabrics assumed to be flow related. This study shows that the vesicles fabrics are related to a sub-horizontal magma flow with the major and minor axes of the vesicles usually on a sub-horizontal or gently dipping plane. The average attitude of x-axis from 3D vesicles shows a value of 26° dipping towards ESE. This integrated study shows that, for narrow dykes, the magnetic lineation is not always the best AMS criteria to define the magma flow vector. Instead, when the magnetic foliation plane is better represented and stable it can be used with good results. These data indicate a magma source located roughly at 3.2 km depth if a linear flow is assumed from the source located at a horizontal distance of 7 km to the sampled sites.

Co-DOPED TITANATE NANOTUBES: EFFECT OF THE STARTING MATERIAL, AUTOCLAVE DWELL TIME AND SYNTHESIS TEMPERATURE ON THEIR MICROSTRUCTURE AND PROPERTIES

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Titanate nanotubes (TNTs) combining the properties of conventional TiO_2 nanoparticles with the properties of layered titanates, have received increasing attention because of their wide potential applications. On the other hand, diluted magnetic semiconductors (DMS) exhibiting ferromagnetic behaviour above room temperature are considered key materials for the development of spintronic devices. Among them, Co-doped TiO_2 oxides are considered very promising materials to achieve such goal.

In this work we report on the synthesis of Co-doped titanate nanotubes via hydrothermal process and on the effect of the starting material, autoclave dwell time and synthesis temperature on their microstructure and properties.

The Co-doped TNTs were characterised by X-ray diffraction (XRD), transmission electronic microscopy (TEM and high resolution TEM) and energy dispersive spectroscopy (EDS). Magnetic properties were measured in the range of 2 K to 320 K, by using a superconducting quantum interference device (SQUID) magnetometer.

SWIFT HYDROTHERMAL METHOD TO PREPARE Co-DOPED TiO_2 ANATASE PHASE NANOPARTICLES

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Since the discovery of ferromagnetism well above room temperature in the Co-doped TiO_2 system, diluted magnetic semiconductors based on TiO_2 doped with transition metals have generated great interest due to their potential use in the development of spintronic devices.
In this work we report on a new and swift chemical route to synthesise highly stable anatase single-phase Co-doped TiO_2 nanoparticles, with dopant concentrations up to 10 at.% and grain sizes ranging between 20 and 30 nm. The crystallographic structure and phase purity of the powders were studied by X-ray diffraction (XRD). The microstructure and morphology of the samples was analysed by transmission electron microscopy (TEM). The average crystallite size was evaluated from XRD data and by TEM image analyses. In order to compare the nominal stoichiometry and the effective Co:Ti ratio, a set of representative samples were analysed by energy dispersive X-ray spectroscopy (EDS) and atomic absorption spectroscopy (AAS). The optical characterization of the powders was carried out by UV-visible diffuse reflectance spectroscopy (DRS) in the wavelength range of 210-830 nm. Their magnetic properties were measured in the range of 4 K to 300 K, by using a superconducting quantum interference device (SQUID) magnetometer.
Complementary structural, microstructural and chemical analyses of the nanopowders synthesised strongly support the hypothesis that a homogenous distribution of the dopant element in the substitutional sites of the anatase structure has been achieved. Moreover, UV-visible diffuse reflectance spectra of powder samples showed red shifts to longer wavelengths/lower energies and band gap energies decreasing with increasing Co concentration, which is consistent with n-type doping of the TiO_2 anatase matrix. Magnetization vs. magnetic field strength hysteresis loops of several samples supports the ferromagnetic behavior at room temperature of the synthesized powders.

Publicado em:
Livros de Resumos da 2nd International Conference on Advanced Nano Materials - ANM 2008, Aveiro, Portugal, 22 a 25 de Junho de 2008.

VANADIUM CATALYSIS FOR THE PARTIAL OXIDATION OF ALKANES UNDER MILD CONDITIONS

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Parcial oxidation reactions of saturated hydrocarbons under mild conditions are expected to provide promising methods towards the use of such unreactive compounds as raw materials for organic syntheses. This general aim constitutes a challenge to modern Chemistry and the field is also of biological significance in view of the ability of a few enzymes to catalyse the partial oxidation of alkanes. Our initial studies by using, as a catalyst, Amavadin, a natural bare vanadium complex with a still unknown biological role, have been extended to other vanadium catalysts which are shown to be particularly active for the following general types of oxidation reactions:

| Peroxidative oxidations of alkanes to alcohols and ketones, typically with aqueous hydrogen peroxidative (a “green” oxidant), at room temperature.

| Oxidation of alkanes with dioxygen (the ideal oxidant) in solvent free systems, by using supported catalysts on modified silica.

Such reactions will also be compared with alkane carboxylations leading to carboxylic acids. Some of the V-systems provide the highest catalytic activity so far reported in the field of alkane functionalization under mild or moderate conditions. They are compared with those based on other metals, and plausible radical mechanisms are discussed on the basis of radical trap and ^{13}C-labelled experiments, and of DFT theoretical studies.

GRAVITY STUDIES IN THE CHAVES AREA

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Entre 1990 e 1992 foi levado a cabo uma grande campanha de levantamento de dados geofísicos no âmbito do projecto "Avaliação dos recursos geotérmicos entre Lamego e Vila Verde da Raia" que tinha com o objectivo o estudo do sistema hidrológico relacionado com as águas termais da zona de Chaves. Esse levantamento compreendeu campanhas de gravimetria, geomagnetismo, resistividade e magnetotelúrica.

Os dados destes levantamentos foram objecto de vários estudos, nomeadamente os apresentados por Moreira *et al.* (1994) e Santos *et al.* (1996, 1997).A área em estudo é caracterizada por uma bacia sedimentar do Quaternário. A bacia foi formada após fracturação das rochas encaixantes (granito e xisto), com a génese de um graben cujo eixo tem direcção NNE-SSW. O levantamento gravimétrico constou de 5200 leituras, com espaçamento entre estações que varia entre os 200m e os 700m, cobrindo uma área de cerca de 1580 km^2. O trabalho de aquisição de dados foi feito, pelo então, Instituto Nacional de Meteorologia e Geofísica. A altitude das estações foi estimada por medição da pressão atmosférica e a localização foi feita em cartas 1/25000 do "Serviço Cartográfico do Exército". Sempre que possível, as medições barométricas foram comparadas com marcos geodésicos. O erro na determinação da altitude será da ordem de 2 m, o que se traduzirá num erro de 0.6 mGal no valor da gravidade, quando se supõe uma densidade de 2.5 g cm^{-3} para a correcção de altitude. Este deverá ser o contributo mais significativo para os erros no cálculo dos valores da gravidade. As correcções de terreno foram efectuadas segundo o método de Hammer. Este é um método muito propenso à geração de erros por se tratar de um método de aplicação manual. Os dados foram apresentados anteriormente por Moreira *et al.* (1994). Para o estudo que aqui se apresenta considerou-se apenas uma área de 175 km^2, cuja distância média de amostragem ronda os 300m. Pode-se verificar que esta carta é dominada por uma estrutura de menor densidade que cruza a área do levantamento de NW a SE. Esta anomalia estará relacionada com uma bacia sedimentar encaixada no granito que caracteriza a região circundante.

Por forma a fazer o mapeamento da anomalia gravimétrica gerada pela bacia de Chaves considerou-se que toda a massa se encontrava concentrada numa camada horizontal com uma espessura definida, denominada camada equivalente. Este método permite delinear os limites da estrutura e evidenciar anomalias dissimulados nas cartas de Bouguer (Murty and Raghavan, 2002).
Assim, considerou-se que a massa se encontra distribuída entre os 10 m e os 150 m de profundidade. Esta camada foi dividida em prismas com 250 m de lado. A densidade de cada prisma foi determinada resolvendo o sistema de equações

$$g_i = \sum_{j=1}^{M} G_{ij} m_j \qquad (1)$$

onde **G** é a matriz de atracção cujas componentes G_{ij} representam a influência que o prisma *j* tem sobre o ponto de leitura *i*. **m** e **g** são os vectores do contraste de densidade dos prismas e dos dados, respectivamente. O sistema foi resolvido utilizando o método dos gradientes conjugados (Press *et al.*, 1992).
Santos *et al.* (1996) apresentou uma análise dos dados de audiomagneto-telúrica obtidos na mesma campanha. Um dos resultados obtidos refere-se ao mapeamento do soco geoeléctrico da bacia sedimentar. De facto, as isopícnicas acompanham as variações de profundidade, verificando-se uma distorção das mesmas nos locais onde a profundidade aumenta. Isto está de acordo com o facto de o enchimento da bacia (sedimentos) ser menos denso do que a rocha do soco (xisto/granito?), o que implicará que, quanto maior a profundidade do soco, maior será o contraste de densidade.
A carta de densidades encontra-se dominada pela grande estrutura do graben com orientação NNE-SSW. No entanto, a observação da carta de profundidades permite identificar outras estruturas com orientação NNW-SSE, as quais são fracamente reflectidas nas isopícnicas.

VIBRAÇÕES NO CORPO HUMANO

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Livro de Resumos do Colóquio Internacional de Segurança e Higiene Ocupacionais - SHO2008, Universidade do Minho, Guimarães, Portugal, 2008.

O termo vibração descreve a oscilação mecânica de um determinado corpo relativamente a um ponto de referência.
Desta forma, o Ser Humano encontra-se diariamente sujeito a vibrações de diferentes tipos, como sejam as experimentadas em casa devido, por exemplo, à passagem de tráfego rodoviário, ferroviário ou aéreo, as experimentadas no transporte entre a casa e o emprego ou, ainda, as vibrações inerentes ao respectivo local de trabalho.
Encontram-se neste último caso as vibrações a que estão sujeitos os trabalhadores que utilizam maquinaria manual do tipo martelos pneumáticos, rebarbadoras, etc. - Vibrações no Sistema Mão-Braço, ou as transmitidas ao corpo do trabalhador como um todo, nomeadamente no caso deste operar sentado em veículos - Vibrações no Corpo Inteiro.
A exposição a Vibrações no Corpo Inteiro pode causar danos físicos permanentes ou distúrbios no sistema nervoso central. Se esta exposição for diária e se estender por um período alargado de tempo (vários anos) pode dar origem a lesões a nível da zona lombar, onde podem surgir deformações da coluna, lombalgias e ciática.
A exposição a Vibrações no Sistema Mão-Braço pode ter consequências mais severas. De facto, a exposição diária a vibrações excessivas durante vários anos pode originar danos físicos permanentes que resultam, normalmente, no denominado Síndrome dos Dedos Brancos, ou em lesões dos músculos e das articulações do pulso e/ou do cotovelo.
Os primeiros sintomas do Síndrome dos Dedos Brancos são o formigueiro, a dormência e a perda de sensibilidade e de controlo nos dedos afectados, que resultam numa afectação séria, não só nas actividades laborais mas também nas de lazer. Mais preocupante ainda é o facto de estes efeitos serem, na maioria das situações, irreversíveis.
As lesões no pulso e/ou no cotovelo são, em geral, resultado de exposições prolongadas a vibrações de baixa frequência, provocadas pela utilização de ferramentas manuais do tipo martelos pneumáticos ou perfuradoras. Estas lesões provocam dores ao nível dos músculos e das articulações do braço determinando perda de força e de controlo.

Desta forma, as vibrações transmitidas ao corpo humano podem, de acordo com a sua severidade e o tempo de exposição, provocar lesões temporárias ou mesmo definitivas, pelo que se tornou indispensável estabelecer critérios relativos à exposição dos trabalhadores às vibrações transmitidas ao Sistema Mão-Braço e ao Corpo Inteiro.
Estes critérios encontram-se consubstanciados na Directiva Europeia 2002/44/CE, de 25 de Junho, cuja transposição para o direito jurídico nacional foi efectuada através do Decreto-Lei nº 46/2006, de 24 de Fevereiro.
Ambos os documentos descrevem a forma correcta de avaliar as vibrações transmitidas ao corpo humano, bem como as acções que devem ser desenvolvidas de forma a atenuar as consequências nefastas para a saúde dos trabalhadores expostos.

NEW C-FUNCTIONALIZED TRIS(PYRAZOLYL)METHANES AND THEIR VANADIUM COMPLEXES

Silva, T.F.S.[1,2]; Wanke, R.[1]; Martins, L.M.D.R.S.[1,3]; Pombeiro, A.J.L.[1]

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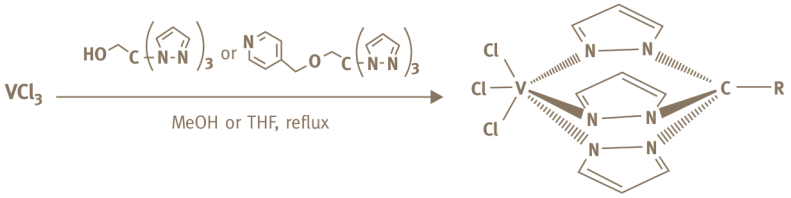
Publicado em:
Livros de Resumos do 6th International Vanadium Symposium, Lisboa, 17 a 19 de Julho de 2008.

Recently, we have initiated the study of the coordination chemistry of hydrotris(1-pyrazolyl)methane, $HC(pz)_3$ (pz = pyrazolyl), and its derivatives bearing substituents on the pyrazolyl rings (*e.g.*, hydrotris(3,5-dimethyl-1-pyrazolyl)methane, $HC(3,5\text{-}Me_2pz)_3$) or the C- methine carbon-substituted tris(1-pyrazolyl)methanesulfonate (as its lithium salt $Li[SO_3C(pz)_3]$), towards V, Fe, Cu or Re centres. In addition, we have found that some of the synthesized scorpionate complexes of those metals can act as selective catalysts in the single-pot oxidation of ethane to acetic acid and in the peroxidative oxidation of cyclohexane to cyclohexanol and cyclohexanone.

Herein we report the study of the reactivity of hydrotris(1-pyrazolyl) methane towards the methine carbon functionalization and the coordination of the obtained C-functionalized scorpionates to a V centre. Hence we have prepared C-functionalized tris(pyrazolyl)methane derivatives $RC(pz)_3$, R= CH_2OH or new $CH_2OCH_2(py)$ (py = pyridyl ring), and investigated their behavior at vanadium(III) centres:



R = $HOCH_2$ or $pyCH_2OCH_2$

The synthesis and characterization of the new scorpionate and V-complexes are reported.

06

MODELLING OF NANO-CONFINED LIQUID CRYSTALS: ORDERING AND ORDERING TRANSITIONS FROM DENSITY-FUNCTIONAL THEORY

Teixeira, P.I.C.[1,2]; Barmes, F.[3]; Anquetil-Deck, C.[3]; Cleaver, D.J.[3]

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Publicado em:
Livro de Resumos da Ìnternational Workshop on Recent Advances in the Understanding of Confined Fluids: from Superfluids to Oil Reservoirs, Abingdon, Reino Unido, Janeiro 2008.

We present a study of the effects of nano-confinement on a system of hard Gaussian overlap particles interacting with planar substrates through the hard-needle-wall potential, extending earlier work by two of us [D.J. Cleaver and P.I.C. Teixeira, Chem. Phys. Lett. **338**, 1 (2001)]. Here, we consider the case of hybrid films, where one of the substrates induces strongly homeotropic anchoring while the other favours either weakly homeotropic or planar anchoring. These systems are investigated using both Monte Carlo simulation and density-functional theory, the latter implemented at the level of Onsager's second virial approximation with Parsons-Lee rescaling. The orientational structure is found to change either continuously or discontinuously depending on substrate separation, in agreement with earlier predictions by others. Theory is seen to perform well in spite of its simplicity, even for small particle elongations.

SIMULATION AND THEORY OF HYBRID-ALIGNED LIQUID CRYSTAL FILMS

Teixeira, P.I.C.[1,2]; Barmes, F.[3]; Anquetil-Deck, C.[3]; Cleaver, D.J.[3]

1 ISEL, Lisboa, Portugal
2 Centro de Física Teórica e Computacional, UL, Lisboa, Portugal
3 Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, United Kingdom

We present a study of the effects of nano-confinement on a system of hard Gaussian overlap particles interacting with planar substrates through the hard-needle-wall potential, extending earlier work by two of us [D.J. Cleaver and P.I.C. Teixeira, Chem. Phys. Lett. **338**, 1 (2001)]. Here, we consider the case of hybrid films, where one of the substrates induces strongly homeotropic anchoring while the other favours either weakly homeotropic or planar anchoring. These systems are investigated using both Monte Carlo simulation and density-functional theory, the latter implemented at the level of Onsager's second virial approximation with Parsons-Lee rescaling. The orientational structure is found to change either continuously or discontinuously depending on substrate separation, in agreement with earlier predictions by others. Theory is seen to perform well in spite of its simplicity, even for small particle elongations.

Publicado em:
Livro de Resumos da 7th Liquid Matter Conference, Lund, Suécia, Junho/Julho 2008.

EFFECT OF THE NUMBER OF SHELLS ON THE PRESSURE AND ENERGY OF TWO-DIMENSIONAL FREE BUBBLE CLUSTERS

Vaz, M.F.[1]; Teixeira, P.I.C.[2,3]; Graner, F.[4]; Cox, S.J.[5]

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Publicado em:
Livro de Resumos da European Conference on Foams 2008, Noordwijk, Holanda, Julho 2008.

We have performed Surface Evolver simulations of two-dimensional hexagonal bubble clusters consisting of a central bubble of area λ surrounded by s shells or layers of bubbles of unit area. Clusters of up to twenty layers have been simulated, with λ varying between 0.01 and 100. In monodisperse clusters (*i.e.*, for λ=1) both the average pressure of the entire cluster and the pressure in the central cell are decreasing functions of s and approach 0.9306 for very large s, which is the pressure in a bubble of an infinite monodisperse honeycomb foam. Here we address the effect of changing the central bubble area λ. For small λ the pressure in the central bubble and the average pressure were both found to decrease with s, as in monodisperse clusters. However, for large λ, the pressure in the central bubble and the average pressure increase with s. The average pressure of large clusters was found to be independent of λ and to approach 0.9306 asymptotically. We have also determined the cluster surface energies given by the equation of equilibrium for the total energy in terms of the area and the pressure in each bubble. When the pressures in the bubbles are not available, an approximate equation derived by Vaz *et al.* was shown to provide good estimations for the cluster energy provided the bubble area distribution is narrow. This approach does not take cluster topology into account. Using this approximate equation, we find a good correlation between Surface Evolver simulations and the estimated values of energy and pressures.

AVALIAÇÃO E FISCALIZAÇÃO EM ACÚSTICA

Rodrigues, Carlos César

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A exigência expressa na legislação aplicável em vigor sobre Poluição Sonora, nomeadamente no Regulamento Geral do Ruído, anexo ao Decreto-Lei nº 9/2007, de 17 de Janeiro, da necessidade de até 2011 se obter a acreditação, pelo Instituto Português de Acreditação, por parte dos Laboratórios responsáveis pela realização de Avaliações Acústicas, determinou uma larga e consistente evolução na qualidade dos resultados das medições acústicas e, consequentemente, das conclusões obtidas.

Por outro lado, as entidades oficiais vêem-se agora na necessidade de manter uma contínua evolução, em termos de aplicação técnico-jurídica, no que à Poluição Sonora diz respeito, já que os seus interlocutores (os Laboratórios Acreditados) estarão, cada vez mais, melhor conhecedores das práticas a aplicar.

Como exemplo, refere-se a situação em que é efectuada uma Avaliação de Incomodidade Sonora, nomeadamente por queixa apresentada em entidade oficial, sem que previamente tenha sido verificado se os requisitos acústicos do edifício em causa cumprem o exigido na legislação aplicável.

De facto, só faz sentido efectuar uma Avaliação de Incomodidade Sonora após o garante de que o Projecto Acústico, em primeiro lugar, e a correspondente obra, em segundo lugar, cumpre os critérios legalmente exigidos. Se a Avaliação de Incomodidade Sonora é efectuada sem o garante da qualidade acústica exigida por lei ao edifício em causa, corre-se o risco de serem imputadas responsabilidades a quem as não tem, com os correspondentes prejuízos financeiros e não só.

Assim sendo, e apesar de se observar, cada vez mais, um maior conhecimento técnico e jurídico por parte de todos os intervenientes em situações em que se exigem Avaliações Acústicas, continua a ser necessário mais formação específica nesta área. A Especialização em Engenharia Acústica da Ordem dos Engenheiros tem pautado a sua actuação de forma a garantir, em termos de Poluição Sonora, a melhor consciencialização dos direitos e deveres da sociedade civil.

Publicado em:
Livro de Resumos das 3as Jornadas de Engenharia Acústica - A Prática da Engenharia Acústica, Ordem dos Engenheiros, Lisboa, Portugal, 2008.

ACÚSTICA DE EDIFÍCIOS vs. INCOMODIDADE SONORA. LICENCIAMENTO E FISCALIZAÇÃO

Rodrigues, Carlos César

ACF - Dept. de Eng. Electrotécnica e Automação, ISEL, Lisboa, Portugal

Publicado em:
Livro de Resumos do Seminário "Medição de Qualidade Térmica e Acústica em Edifícios", Universidade do Algarve, Faro, Portugal, 2008.

Os dados disponíveis mostram, de forma clara, que as Reclamações por Incomodidade devida ao Ruído têm vindo a aumentar de forma significativa ao longo dos últimos anos. Assim sendo, é indispensável que as Autoridades com competência em matéria de Poluição Sonora consigam fiscalizar adequadamente se a Reclamação do queixoso se deve a um aumento do ruído produzido pelo eventual prevaricador ou se, pelo contrário, é o Isolamento Sonoro em causa (a sons por condução aérea e/ou a sons por condução estrutural) que é insuficiente.

Deve, então, analisar-se as Situações de Incomodidade devidas ao Ruído antes ou após a verificação de que os Requisitos Acústicos dos Edifícios se encontram cumpridos? É que quer a Incomodidade Sonora, quer a Acústica dos Edifícios, está devidamente regulamentada em Portugal através, respectivamente, do Decreto-Lei nº 9/2007 e do Decreto-Lei nº 129/2002.

SISMO 1998 – AÇORES: UMA DÉCADA DEPOIS

Capítulo 05: Estudos Específicos com redes sísmicas para caracterização sísmica de pormenor

Dias, N.A.[1,2]; Matias, L.[3]

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Edição: SPRHI, S.A., Horta
ISBN: 978-989-20-1223-0
Data de Publicação: Julho 2008; pg. 89-98

The Azores archipelago (Portugal) is located on an oceanic plateau, in a geodynamic environment prone to intense seismic and volcanic activity. The July 9th 1998 earthquake, located offshore of NE Faial Island, triggered an aftershock sequence of thousands of events that lasted for several months. Following the main shock, 7 portable seismic stations were deployed by IM and CGUL/IGIDL in the islands of Faial, Pico and S. Jorge to increase the coverage of the seismic crisis by the permanent seismological network of SIVISA. The increased monitoring capability of the network allowed for the first time coverage with modern instruments of a seismic crisis in the Azores. This allowed the characterization of the observed seismicity (occurrence rates, main seismogenic structures identification, type of sources) and of the crustal structure of this region (type of Lithosphere, 1-D and 3-D modeling, crustal stresses, distribution of fractures). In this work we will resume some of the results obtained (Dias *et al.*, 2007; Matias *et al.*, 2007).

In order to investigate the crustal structure in this region, we have conducted a local earthquake tomography study in the area of the islands of Faial, Pico and S. Jorge using the data recorded in July 1998. A new 1-D velocity model FAIAL98 was derived showing a heterogeneous upper crust, testified by the observed differences in site effects at the stations, while the middle crust from ~2.5 to 8 km depth is quite homogeneous. The Moho is located at about 12-13 km depth and the Vp/Vs ~ 1.78.

Based on the new 1-D model, a tomographic inversion was also performed attaining a 3-D model of the Vp and Vp/Vs crustal structure. In the upper crustal layers, consistency is seen between the tomographic results and the islands' surface volcanic units. Beneath the Faial central volcano a low Vp (‹6.0 km/s) anomaly roughly located at 3-7 km depth, suggests a connection to the plumbing system, possi-

bly the presence of a magma chamber. In NE Faial, a high Vp (›6.3 km/s) body was found located at mid-lower crust, most likely an intrusion of gabbroic composition, that is bordered by the registered seismic activity; its shape suggesting a tectonic controlled mechanism. The estimated crustal thickness under the islands volcanic buildings was ~14 km.

The new hypocentral solutions obtained from the 1-D and 3-D inversions show that the events are mainly concentrated in the middle-lower crust (8-12 km depths) while their spatial distribution shows a main cluster trending SSE. This direction of elongation is consistent with one of the fault planes (N151ºE) of the Harvard-CMT solution for the main shock. The aftershocks pattern shows that several fault systems were reactivated by the main shock. Besides the two main tectonic directions, trending WNW-ESE and NNW-SSE observed inland at Faial, Pico and S. Jorge, there is also evidence of a new tectonic direction trending WSW-ENE.

The presence of seismic anisotropy compatible with the EDA model has been confirmed beneath some of the stations, with a correlation between the distribution of fractures and the location of each station. The direction obtained for the maximum compressive stress from the shear-waves polarization, together with the same direction retrieved from single and composite focal mechanisms, shows a complex stress pattern: the expected direction roughly NW-SE rotates to SW-NE in the eastern sector of Faial Island and extending to the NW marine events. The thicker crust obtained for the Faial-Pico area, as compared to a "typical" oceanic crust, is due to a thickening of the layer 3, an indicator of a high magmatic budget that cooled and crystallized in depth, the extrusive volcanism rate having a normal significance in the crustal building process. The high-seismic velocity body detected NE of Faial and bordered by the area of highest seismic activity, interpreted as a mafic-ultramafic intrusion (mainly Gabbros), corroborates this hypothesis. The seismicity distribution together with the rotation observed in the stress directions show that this body played a major role in the tectonic control of the seismic sequence of 1998.

BIOMIMETIC AND SUPRAMOLECULAR SYSTEMS

Godinho, M.H.[1]; Figueirinhas, J.L.[2,3]; Brogueira, P.[3,4]; Teixeira, P.I.C.[5,6]

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6 C. de Física Teórica e Computacional, UL, Lisboa, Portugal

Edição: Nova Science Publishers; Capítulo: Tuneable micro- and nanoperiodic structures in urethane/urea networks
ISBN: 978-1-60456-405-1
Data de Publicação: Setembro 2008; pg. ?-?

Micro- and nano-patterned materials are of great importance for the design of new nanoscale electronic, optical and mechanical devices, ranging from sensors to displays. A prospective system that can support a designed functionality is elastomeric polyurethane thin films with nano- or micro-modulated surface structures ("wrinkles"). These wrinkles can be induced on different lengthscales by mechanically stretching the films, without the need for any sophisticated lithographic techniques. In the present article we focus on the experimental control of the wrinkling process. A simple model for wrinkle formation is also discussed, and some preliminary results reported. Hierarchical assembly of these tunable structures paves the way for the development of a new class of materials with a wide range of applications, from electronics to biomedicine.

CLORO-COMPLEXOS ESCORPIONATOS DE FERRO E VANÁDIO E SUA APLICAÇÃO COMO CATALISADORES DA OXIDAÇÃO PARCIAL, EM CONDIÇÕES SUAVES E AMBIENTALMENTE TOLERÁVEIS, DE CICLO-HEXANO A CICLO-HEXANOL E CICLO-HEXANONA

Pombeiro, A.J.L.[1]; Martins, L.M.D.R.S.[1,2]; Alegria, E.C.B.A.[1,2]; Silva, T.F.S.[1,3]

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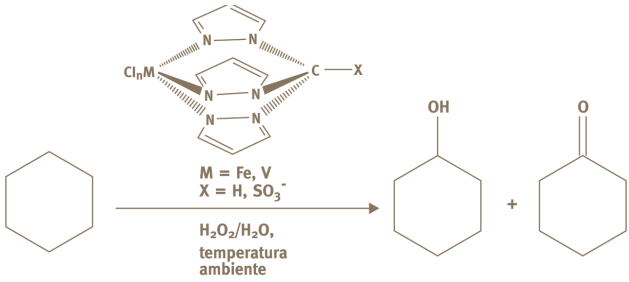
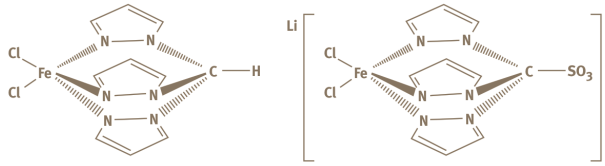
Patente Número: PT 104153
Data de Apresentação Internacional (Nacional): 04 de Agosto de 2008
Data de Publicação: Pendente

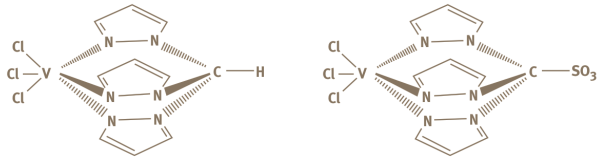
A invenção refere-se a novos cloro-complexos escorpionatos de ferro e vanádio, de fórmulas (1) a (4), e ao uso daqueles compostos e de complexos relacionáveis como catalisadores da oxidação peroxidativa do ciclo-hexano a ciclo-hexanol e ciclo-hexanona, com elevados rendimento e selectividade, realizada em condições suaves e ambientalmente toleráveis, em particular em meio aquoso.





[FeCl2{HC(pz)3}]
1

Li[FeCL2{SO3C(pz)3}]
2



[VCl3{HC(pz)3}]
3

[VCl3{SO3C(pz)3}]
4

ANÁLISE DE LIMITES AO ESPAÇO DE PARÂMETROS DE MODELOS SUPERSIMÉTRICOS DE QUEBRA DE SIMETRIAS DE CARGA E DE COR

Pereira, Paulo

Mestrado em: Física
Grau Concedido por: Universidade de Lisboa
Orientadores: António Amorim e Pedro Ferreira
Provas Concluídas em: 18 de Dezembro de 2008

Foi feita uma análise numérica aprofundada do espaço de parâmetros supersimétrico, e a importância que mínimos com quebra de carga ou cor podem ter para impor restrições a esse espaço.

NOVOS COMPLEXOS ESCORPIONATOS DE VANÁDIO E COBRE CATALISADORES DA OXIDAÇÃO DE ALCANOS

Silvério da Silva, Telma Filipa

Mestrado em: Engenharia Química
Grau Concedido por: Instituto Superior de Engenharia de Lisboa
Orientadores: Luísa Margarida Dias Ribeiro de Sousa Martins
Provas Concluídas em: 28 de Novembro de 2008

Neste trabalho foi descrita a síntese e caracterização estrutural dos seguintes novos compostos de vanádio ou de cobre com os ligandos azotados escorpionatos hidrotris(1-pirazolil)metano ou tris(1-pirazolil) metanossulfonato: $[VCl_3\{HC(pz)_3\}]$, $[VCl_3\{SO_3C(pz)_3\}]$, $[CuCl_2\{HC(pz)_3\}]$, $[CuCl\{SO_3C(pz)_3\}]$ e $[Cu\{HC(pz)_3\}_2]Cl_2$.
Investigou-se a actividade catalítica destes compostos na carboxilação do metano e do etano aos ácidos carboxílicos correspondentes, num só "passo", e na oxidação peroxidativa do ciclo-pentano e do ciclo-hexano, originando os álcoois e cetonas correspondentes, em condições suaves.

06


07

MATEMÁTICA

Anuário Científico 2008

ISEL

PLATE EIGENFREQUENCY OPTIMIZATION WITH GENETIC ALGORITHMS AND RANDOM KEYS

Aguilar Madeira, J.F.[1,2]; Pina, H.L.[1]; Rodrigues, H.C.[1]

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2 Departamento de Matemática, DEETC-ISEL, Lisboa, Portugal

Topology optimization consists on finding the spatial distribution of a certain amount of material so that the resulting structure to has some optimal property, for instance, maximization of the eigenfrequencies, a topic currently object of intense research.
In this paper we develop a method based on trees to generate initial feasible individuals that remain feasible upon crossover and mutation and as such do not require any repairing operator.
As application example we study the topology optimization of structures where the objective functions is the maximization of the first and the second eigenfrequencies of a plate. All cases having a prescribed material volume constraint.

Publicado em:
Actas do The Sixth International Conference on Engineering Computational Technology, Athens, Greece, September, 2008.

POPULATIONAL GROWTH MODELS IN THE LIGHT OF SYMBOLIC DYNAMICS

Aleixo, S.[1,4]; Rocha, L.[2,4]; Pestana, D.[3,4]

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2 Dept. de Engenharia Química, ISEL, Lisboa, Portugal
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4 C. de Estatística e Aplicações da Universidade de Lisboa, Lisboa, Portugal

Using symbolic dynamic thecniques, populational growth models proportional to beta densities, are investigated. Our results give explicit methods to investigate the chaotic behaviour of populational growth models, when the malthusean parameter increases. The chaotic complexity is measured in terms of the topological entropy.

Publicado em:
Proceedings of the ITI 2008, 30th International Conference on Information Technology and Interfaces, Cavtat, Croácia, Junho de 2008, pp. 311-316.

FAMÍLIA PARAMETRIZADA GLE

Aleixo, S.[1,3]; Diamantino, F.[2,3]; Pestana, D.[2,3]

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2 Dept. de Estatística e Investigação Operacional, FCUL, Lisboa, Portugal
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Neste trabalho descrevermos as propriedades estruturais importantes e os métodos usados para gerar números pseudo-aleatórios com a distribuição Gaussiana-Laplace Estendida (GLE). Publicámos electronicamente, em www.ceaul.fc.ul.pt, listagens de pseudo-aleatórios GLE, para valores adequados do parâmetro de forma.

Publicado em:
Notas e comunicações do CEAUL, Nota nº 15 – Lisboa, Setembro de 2008.

NUMERICAL SIMULATION OF A VISCOELASTIC FLUID WITH A PRECONDITIONED SCHWARZ METHOD

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2 CEMAT, Departamento de Matemática, IST, Lisboa, Portugal

Publicado em:
Polish Academy of Sciences, Institute of Mathematics, Banach Center Publications, Parabolic and Navier Stokes Equations, vol. 81 part 1, pp.65-80.

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 nonlinear system of partial diferential equations decoupled into a Navier-Stokes system and a tensorial transport equation. Using a modified Schwarz algorithm, involving block preconditioners for 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.

SYMBOLIC DYNAMICS AND CHAOTIC SYNCHRONIZATION IN COUPLED DUFFING OSCILLATORS

Caneco, A.[1,4]; Grácio, C.[2,4]; Leonel Rocha, J.[3]

1 Dept. de Engenharia de Electrónica e Telecomunicações e de Computadores, ISEL, Lisboa, Portugal
2 Dept. de Matemática, Universidade de Évora, Évora, Portugal
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In this work we discuss the complete synchronization of two identical double-well Duffing oscillators unidirectionally coupled, from the point of view of symbolic dynamics. Working with Poincaré cross-sections and the return maps associated, the synchronization of the two oscillators, in terms of the coupling strength, is characterized. We obtained analytically the threshold value of the coupling parameter for the synchronization of two unimodal and two bimodal piecewise linear maps, which by semi-conjugacy, under certain conditions, gives us information about the synchronization of the Duffing oscillators.

Publicado em:
Journal of Nonlinear Mathematical Physics, 2008, 15, 102-111.

07

CHAOTIC SYNCHRONIZATION OF PIECEWISE LINEAR MAPS

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2 Dept. de Matemática, Universidade de Évora, Évora, Portugal
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Publicado em:
World Scientific Publishing Co, International Conference on Difference Equations and Applications (ICDEA), 23 a 27 Julho 2007, em Lisboa, Portugal.

We derive a threshold value for the coupling strength in terms of the topological entropy, to achieve synchronization of two coupled piecewise linear maps, for the unidirectional and for the bidirectional coupling. We prove a result that relates the synchronizability of two m-modal maps with the synchronizability of two conjugated piecewise linear maps. An application to the bidirectional coupling of two identical chaotic Duffing equations is given.

GRAPHS, SYMBOLICS DYNAMICS AND SYNCHRONIZATION OF NETWORKS

Caneco, Acilina[1,4]; Fernandes, Sara[2,4]; Grácio, Clara[2,4]; Leonel Rocha, J.[3]

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In this work we establish the relation between some graph parameters, particularly, clustering coefficients and conductance, with the network synchronization. There is a recent interest in the study of how the parameters relating the topology of the graph affect the synchronizability of the network associated with the graph. There are known formulas relating some graph invariants with the Laplacian eigenvalues that are relevant to the synchronizability of the network, but none for the clustering coefficient. So, we address our work to the study of the effect of clustering in the amplitude of the synchronization interval.

Publicado em:
Dynamics & Applications, 08 a 12 Setembro 2008, em Braga, Portugal.

NONLINEAR MAXIMUM PRINCIPLES AND APPLICATIONS

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We extend a nonlocal maximum principle obtained in a previous paper, which allows us to use a monotone method to find radial solutions of an elliptic problem in the presence of lower and upper solutions.

Publicado em:
Communications on Applied Nonlinear Analysis, Vol.15, No. 1, January, 2008, pp. 1-17.

SECOND ORDER NON-AUTONOMOUS HOMOCLINICS

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We study the existence of positive solutions for a second order differential equation, with boundary conditions u'(0)=u(+∞)=0. The main motivation is to check that some well known results concerning the existence of homoclinics for the autonomous case extend to the non-autonomous equation.

Publicado em:
Livros de Resumos da Conferência Mathematical Models in Engineering, Biology and Medicine, 16 a 19 de Setembro de 2008.

COMMUTATIVE JORDAN ALGEBRAS PILING – APPLICATION TO STEP NESTED DESIGNS

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Let $T^2_{i=l}$ M_i be the family of matrices $D(B_1,B_2)$ with $B_l \in$, M_l, l=1,2. If M_1 and M_2 are commutative Jordan algebras $T^2_{i=l}$ M_i will be a commutative Jordan algebra. The properties of this binary operations are studied and it is applied to step nested designs.

Publicado em:
Livros de Resumos do 17th International Workshop on Matrices and Statistics, Tomar, 23 a 26 de Julho de 2008.

THREE-WAY CROSSED CLASSIFICATION WITH INTERACTION

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In many fields of research, an investigator often Works with experiments or surveys involving three or more factors, which entails simultaneous data collection under conditions determined by several factors. This type of design is usually more economical and can provide more information than separate one-way or two-way layouts.

Publicado em:
Livros de Resumos do 3rd Workshop on Statistics, Mathematics and Computational and 1st Portuguese-Polish Workshop on Biometry, Lisboa, 21 e 22 de Julho de 2008.

FIDUCIAL INFERENCE WITH AND WITHOUT PIVOT VARIABLES

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This work describes the general principles of the fidutial inference. A brief survey of it's competing inferencial theories as well as a comparison with them are also provided.

Publicado em:
Livros de Resumos do 3rd Workshop on Statistics, Mathematics and Computational and 1st Portuguese-Polish Workshop on Biometry, Lisboa, 21 e 22 de Julho de 2008.

THE DEPENDENCE OF THE TARGET EROSION DEPTH ON THE DIRECTION OF MAGNETIC INDUCTION IN A PLANAR MAGNETRON DISCHARGE

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The target erosion depth, *h (r)*, is measured along a radius of a circular magnetron target and the magnetic induction vector is mapped.
A simplified model of the discharge is developed in the present work. The model shows that the erosion depth along a target radius is well defined by a relation of the type, $h(r) = h_m [1 - \exp(-b \cot\theta(r,L))]$, where h_m is the maximum target erosion depth, b is a characteristic parameter of the discharge, L is the thickness of the cathode sheath and θ the angle made by the magnetic induction and the target surface.
The relation obtained for the dependence of the target erosion depth on the direction of the magnetic induction fits well the experimental results.

Publicado em:
RIVA, 7th International Conference of Vacuum, Monte de Caparica, Portugal, June 22nd, 2008- June 25th, 2008.

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MÉTODO DOS ELEMENTOS FINITOS: ANÁLISE, SOFTWARE, E APLICAÇÕES EM ENGENHARIA

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Publicado em:
Actas do "5º Congresso Luso-Moçambicano de Engenharia", ISBN: 978-972-8826-19-2, 2008, artigo convidado, pp. 771-772.

O Método dos Elementos Finitos (MEF) é desde há mais de 50 anos, um dos procedimentos de cálculo mais utilizado para a resolução de "problemas contínuos" em Engenharia. Estes problemas, governados por complexos sistemas de equações com derivadas parciais, sujeitos a condições específicas, requerem soluções numéricas adequadas baseadas no MEF.
Usando exemplos, com desenvolvimentos teóricos e computacionais, apresentaremos uma descrição de outro tipo de problemas importantes que actualmente se estudam em Engenharia, referindo as estratégias numéricas de resolução usando o MEF.

LABORATÓRIO VIRTUAL DE MATEMÁTICA EM PLATAFORMA MOODLE

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Com este trabalho propomos apresentar práticas de b-learning desenvolvidas no contexto do ensino da Matemática no curso de Engenharia Civil, no ISEL. Mostraremos também, a forma como estas práticas consubstanciadas com a implementação de um laboratório virtual de matemática instalado na plataforma Moodle, contribuem para uma melhoria da qualidade de ensino nas disciplinas de Análise Matemática I e Análise Matemática II, do curso de Engenharia Civil.

Publicado em:
Actas do "II Encontro de Comunidades de Aprendizagem Moodle", ISBN: 978-989-95925-0-6, 2008, pp. 126-131.

INVARIANTYS OF TEMPLATES, KNOTS AND LINKS GENERATED BY RENORMALIZABLE LORENZ MAPS

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We describe the sub-Lorenz templates generated by renormalizable Lorenz maps, in terms of the templates generated by the renormalized map and by the map that determines the renormalization type. Consequently we obtain explicit formulas for the Williams ζ function of renormalizable sub-Lorenz templates and also for the genus and the braid index of renormalizable Lorenz knots and links.

Publicado em:
Livros de Resumos da Conferência Dynamics and Applications, in honour of Mauricio Peixoto and David Rand, Universidade do Minho, Braga, Portugal.

EFFECTIVE COMPUTATION OF THE MULTIVARIABLE ALEXANDER POLYNOMIAL OF LORENZ LINKS

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Given two different representations of a Lorenz link, we compare how they affect the computation of the multivariable Alexander polynomial. We also compare the Alexander polynomial with the trip number and genus. Our experimental results lead us to conjecture that, for Lorenz knots, the Alexander polynomial is an equivalent invariant to the pair (trip number, genus). Finally, we give a counterexample in the case of Lorenz links.

Publicado em:
Physica D: Nonlinear Phenomena, Volume 237, Issue 24, 15 December 2008, pages 3322-3328.

CURSO DE ANÁLISE MATEMÁTICA: CÁLCULO EM IR^n

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Este livro foi pensado para tornar acessiveis os conceitos de Análise Matemática especialmente nas licenciaturas de Engenharia, desenvolvendo competências de manipulação dos métodos matemáticos de maior relevância nesse contexto.
Tornando o leitor parte activa no proceso de aprendizagem, cada um dos capítulos aborda um desenvolvimento específico do tema em estudo, ilustrando-o com vários exemplos indicativos das suas aplicações mais importantes e adicionando diversos exercícios práticos da maior utilidade para esclarecer e consolidar os conteudos teóricos apresentados.

MÉTODOS ANALÍTICOS EM PROBABILIDADES E MÉTODOS PROBABILÍSTICOS EM ANÁLISE: FRACTALIDADE ASSOCIADA AOS MODELOS BETA(p,q), EVOLUÇÃO DE POPULAÇÕES E DIMENSÕES DE HAUSDORFF

Aleixo, Sandra Maria da Silva Figueiredo

Doutoramento em: Estatística e Investigação Operacional
Grau Concedido por: Universidade de Lisboa
Orientadores: José Leonel Linhares da Rocha e Dinis Duarte Ferreira Pestana
Provas Concluídas em: 9 de Dezembro de 2008

Deduziram-se modelos de crescimento populacional proporcionais a densidades beta com parâmetros de forma p e 2, onde $p > 1$, cuja complexidade dinâmica está relacionada com o parâmetro malthusiano r. Usando técnicas de dinâmica simbólica, investigou-se o comportamento caótico destes modelos, em termos de entropia topológica, no espaço de parâmetros (r,p), identificando diferentes comportamentos dinâmicos.
Verificou-se a universalidade da constante de Feigenbaum nos modelos apresentados, usando uma fórmula diferente daquela que é usualmente apresentada na literatura.
O efeito de Allee foi analisado nestes modelos. Para $p > 2$, eles exibem uma dinâmica populacional onde o efeito de Allee surge naturalmente. No entanto, no caso onde $1 < p \leq 2$, os modelos propostos não incluem este efeito. Para invocá-lo, apresentaram-se alguns modelos alternativos e investigaram-se as suas dinâmicas. Analisou-se também a negatividade da derivada de Schwarz em todos os modelos propostos.
Definiu-se poeira de Cantor aleatória, um fractal obtido por eliminação recursiva do espaçamento central que é definido entre o mínimo e máximo de duas observações aleatórias uniformemente distribuídas, de cada intervalo da iteração anterior. A designação atribuída ao fractal é justificável, uma vez que os valores esperados dos extremos dos intervalos de cada iteração, coincidem com os extremos dos intervalos da correspondente iteração na construção da poeira de Cantor determinista.
Calculou-se a dimensão de Hausdorff (que intuitivamente avalia a que ponto um conjunto é denso) da poeira de Cantor aleatória, e verificou-se que apesar de a poeira de Cantor ser o "fractal médio", da poeira de Cantor aleatória, é mais denso (a dimensão de Hausdorff da poeira de Cantor C é superior dimensão de Hausdorff da poeira de Cantor aleatória F).
Este resultado levou-nos a uma definição mais geral de conjuntos de Cantor aleatórios FX, com X tendo distribuição Beta(p,q), ao cálculo das suas dimensões de Hausdorff, e das dimensões de Hausdorff dos

fractais deterministas que são a esperança daqueles fractais aleatórios, num sentido similar ao de a poeira de Cantor determinista ser a esperança da poeira de Cantor aleatória.
O fenómeno é geral, e para essa diferença entre dimensões de Hausdorff encontrou-se uma explicação probabilista que reforça a interpretação de dimensão de Hausdorff como reveladora da abundância de pontos do fractal.

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