# CONFERENCE PROGRAM

**Monday, 5th September**

**Plenary 1**
1. Separation Process Development  
   *Phillip C. Wankat*

**Plenary 2**
3. On the complexity of virus-host cell interaction: dynamics of influenza A virus replication in mammalian cell culture  
   *Udo Reichl*

**Session 1: Methods and tools for managing the complexity**
4. Metabolomics as a tool to understand E. coli metabolic responses in recombinant processes  
   *Carneiro, Sónia; Ferreira, Eugénio C.; Rocha, Isabel*

   *Costa, Diogo Moreira; Martins, Fernando Gomes; Melo, Luís Manuel Ferreira de*

   *Lopes, Rodrigo JG; Quinta-Ferreira, Rosa M*

10. Modelling key performance parameters of an MBR for wastewater treatment  
    *Galinha, Claudia; Carvalho, Gilda; Portugal, Carla A. M.; Reis, Maria A. M.; Crespo, João G.*

12. A New MILP Model for the Optimal Design of Industrial Water Networks  
    *Teles, João P.; Castro, Pedro M.; Matos, Henrique A.*

**Session 2: Bioresources and bioenergy**
14. Greenhouse gas life cycle for Fossil and Renewable Diesel  
    *Caeiro, Ana Margarida; Brozou, Nikolaos*

15. MgAl hydrotalcites as solid heterogeneous catalysts for biodiesel production  
    *Gomes, João Fernando; Pina, Jaime Filipe; Gonçalves, Líssia; Bordado, João Carlos*

17. BIODIESEL PRODUCTION FROM HIGH ACIDITY INDUSTRIAL BY-PRODUCTS USING HETEROGENEOUS CATALYSIS  
    *Soares Dias, Ana Paula; Domingues, Carina; Carvalho, Renato; Bordado, João; Henriques, Carlos; Neiva Correia, Joana*

19. Application of Response Surface Methodology in predicting liquids yields from the pyrolysis of waste mixtures  
    *Paradelo, Filipe Manuel; Pinto, Filomena; Ramos, Ana Maria; Gulyurtlu, Ibrahim*

21. Valorization of a side product of pulp industry under the concept of Biorefinery  
    *Pereira, Susana R; Fernandes, Daniel L A; Silva, Carlos M; Serafim, Luísa S; Evtyugin, Dmitry; Xavier, Ana M R Barreto*

23. Enzymatic hydrolysis of pretreated primary sludge from a Portuguese pulp and paper mill  
    *Mendes, Cátia Teixeira; Rocha, Jorge Manuel; Carvalho, Maria Graça*

**Session 3: Chemical and biological process-product engineering**
25. Introducing olfaction into Product Engineering  
    *Teixeira, Miguel A.; Rodríguez, Oscar; Rodrigues, Alírio E.*

27. Multivariate SPC / EPC Integration in MIMO Dynamic Processes  
    *Moita, Raquel D; Rato, Tiago J; Santos, Lino O; Saraiva, Pedro M; Seabra dos Reis, Marco*
Impact of reverse osmosis on the electro-oxidation of cytotoxic compounds: effect of ionic composition and strength
Oliveira, Patrícia Isabel; Velizarov, Svetlozar Gueorguiev; Crespo, João Goulão; Portugal, Carla Moreira

Octane Upgrading of TIP Processes by Recycling in a Layered Zeolite 5A/BETA PSA
Correia Silva, José António; Bácia, Patrick; Rodrigues, Alírio

The NETmix reactor: characterization and quantification of mixing
Gomes, Paulo Jorge; Dias, Madalena M.; Lopes, Jose Carlos

Plenary 3

Bioresources and Bioenergy: about hypes and mavericks
Willy Verstraete

Poster session 1: Methods and tools for managing the complexity

Pilot-scale constructed wetlands hydrodynamics modelling from tracer experiments
Mateus, Dina M. R.; Fernandes, Carina I. A.; Almeida, Marina M. P.; Pinho, Henrique J. O.

Study on the toxicological effects of airborne nanoparticles from welding processes
Gomes, João Fernando; Albuquerque, Paula Cristina; Miranda, Rosa Maria; Vieira, Teresa Maria

An ordinal regression method to customer prioritization requirements in chemical product design
João, Isabel Maria; Silva, João Miguel

Determination of Operating Conditions in the Alkylation Process using the Firefly Algorithm and the Levenberg Marquardt Algorithm
Lobato, Fran Sérigo; Souza, Davi Leonardo de; Almeida, Gustavo Matheus de

Aflatoxin B1 in peanuts: development of an alternative chromatographic method
Alves Silvério, André; Lopes, Maria Manuel

Fault detection in the Tennessee Eastman process using integrated dynamic principal components analysis and missing data methods
Rato, Tiago Janeiro; Reis, Marco Seabra

Modelling molecular and inorganic data of Amanita ponderosa mushrooms using artificial neural networks
Salvador, Cátia Sofia; Martins, M. Rosário; Vicente, Henrique; Neves, José; Arteiro, José M.; Caldeira, A. Teresa

The role of the sensitivity analysis and optimization criterion on kinetic parameter determination in anaerobic digestion
Donoso-Bravo, Andres; Mailier, Johan; VandeWouwer, Alain

Theoretical and Experimental Study of Acetic Acid Esterification
Antunes, Bruno Manuel; de Portugal, Maria Inês; Silva, Carlos Manuel

State and input estimation in phytoplanktonic cultures using a stochastic inverse
Rocha-Cózatl, Edmundo; Moreno, Jaime; Vande Wouwer, Alain

Combining dielectric and thermal characterization techniques for studying the molecular dynamics of a pharmacutical drug: S-ibuprofen
Rodrigues, Andreia Filipa Costa; Víciosa, Maria Teresa; Correia, Natália Teixeira

Time versus accuracy: truncation effects on the theoretical study of the Jacobsen catalyst
Teixeira, Filipé; Melo, André; Freire, Cristina; Cordeiro, M. Natália

Stabilizing NMPC for Distributed Process System with Fluid Flow
Costa, Sérgio Jorge; Igreja, José Manuel

Genetic Characterization of Yam Cultivars (Colocasia esculentaL. Schott) Preserved in Germplasm Banks
REBOUÇAS, TIYOKO NAIR HOJO; CASAES, RAQUEL; PINHATI, FERNANDA ROMANHOLI; SILVA, JOAB TRAJANO; PASCHOALIN, VANIA FLSIO

Interaction study of viruses with an ion exchange matrix: a scale down tool
Nestola, Piergiuseppe; Peixoto, Cristina; Mota, José P.B.; Carrondo, Manuel J.T.; Alves, Paula M.

Combining metabolic and proteomics inputs for improved bioprocess performance: the baculovirus-insect cell system as a case study
Carinhas, Nuno Eduardo; Bernal, Vicente; Carrondo, Manuel José Teixeira; Jenoe, Paul; Oliveira, Rui; Alves, Paula Marques
Octane Upgrading of TIP Processes by Recycling in a Layered Zeolite 5A/BETA PSA

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With the increasing regulation of gasoline composition, paraffin isomerization has grown rapidly in importance as a means to boost light naphtha research octane number (RON). Isomerization of light naphtha fractions rich in $n$C5 and $n$C6 is achieved by catalytic reaction on either chlorinated alumina or zeolite based Pt-containing catalysts which convert the low octane linear paraffins into branched ones. Several variations of the $n$C5/$n$C6 isomerization process are commercially available. In once-through isomerization, i.e. without recycle of the isomerate product, a product RON up to 80 can be achieved. If the normal paraffins in the reactor product are separated and recycled the product RON can be improved up to 88-89. For such recycle units the octane quality of the final isomerate product depends on the separation technique applied. The octane gain from pentanes and hexanes can be controlled by the Deisopentanizer (DIP) and Deisohexanizer (DIH) distillation columns, respectively. The separation between $n$- and iso-paraffins is also possible by selectively adsorbing the normal paraffins on a molecular sieve bed of zeolite 5A (e.g., the Ipsorb process from Axens and the Total Isomerization Process (TIP) from UOP). The second option is from afar the less energy consuming recycle technology available.

The objective of this work consists in studying the separation mono/dibranched paraffins by cyclic adsorption process using a layered bed of zeolites 5A and Beta (Figure 1). Aspen ADSIM 2006.5 (AspenTech Inc.) was used for numerically solving an adiabatic dynamic model incorporating mass, energy and momentum balance. Model parameters were taken from experimental data reported in the literature\textsuperscript{1,2}. Parametric studies were simulated to determine how process performance is affected by purge quantity, 5A-to-Beta ratio, repressurization/blowdown schemes and operating temperature. Figure 2 shows that a combination of zeolites 5A and Beta can produce an octane gain of 1 RON at 523 K comparatively to the conventional TIP\textsuperscript{3} by reducing the monobranched C6 fraction in the product. Another advantage of this configuration is the possibility to increase the penetration distance because zeolite Beta acts like a “barrier” to the linear alkanes desorbed from zeolite 5A during the co-current depressurization step. It was also demonstrated that a slight increase in temperature (20 K) results in a RON benefit of 0.2 points. Several alternatives are provided to improve the performance of the existing TIP processes with this combination of adsorbents.
Figure 1. Improvement of TIP process in a layered 5A/BETA PSA.

Figure 2. RON product as a function of zeolite 5A mass fraction and purge-to-feed volumetric ratio in a layered 5A/BEA PSA. $T = 523K$; $P_{\text{Feed}}/P_{\text{Purge}} = 5/1$ bar; pressurization with feed; co-current depressurization; pure $H_2$ purge; $t_{\text{cycle}} = 200$ s.

References:

