



**2<sup>nd</sup> DOCTORAL CONGRESS  
in ENGINEERING**

**8 - 9 JUNE 2017 • FEUP • PORTO • PORTUGAL**

# **Book of Abstracts**



*2<sup>nd</sup> Symposium on Chemical,  
Biological and Environmental Engineering*



# **Book of Abstracts**

of the

## **2<sup>nd</sup> Symposium on Chemical, Biological and Environmental Engineering**

**Editors:**

Alexandra Pinto, Daniel Direito, Helder X. Nunes,  
Joana Vilas Boas, Marta Barbosa, Sara Ramos

Porto  
June 2017

This volume contains the abstracts presented at the Symposium on Chemical, Biological and Environmental Engineering, within the 2<sup>nd</sup> Doctoral Congress in Engineering - DCE17, held in Porto, between June 8<sup>th</sup> and 9<sup>th</sup>, 2017.

**Title:** Book of Abstracts of the 2<sup>nd</sup> Symposium on Chemical, Biological and Environmental Engineering

Edited by **Alexandra Pinto, Daniel Direito, Helder X. Nunes, Joana Vilas Boas, Marta Barbosa, Sara Ramos**

**Published by:**

FEUP Edições

<http://fe.up.pt/dce17/symposia/symposium-on-chemical-biological-and-environmental-engineering/BoAChemBioEnvEng.pdf>

First edition June 2017

ISBN. 978-972-752-218-7

Universidade do Porto, Faculdade de Engenharia, Departamento de Engenharia Química, Rua Dr. Roberto Frias s/n 4200-465 Porto, Portugal

Copyright © FEUP

# **Symposium Committee**

## **Scientific Committee**

**Chair: Alexandra Pinto | FEUP**

Arminda Alves | FEUP

Carmen Rangel | LNEG

Cidália Botelho | FEUP

Daniel Direito | FEUP

Fernando Pereira | FEUP

Filomena Barreiro | IPB

Francisco Malcata | FEUP

Helder Xavier Nunes | FEUP

Joana Vilas Boas | FEUP

José Teixeira | U.Minho

Manuel Alves | FEUP

Manuel Simões | FEUP

Marta Barbosa | FEUP

Miguel Madeira | FEUP

Sara Ramos | FEUP

## **Organizing Committee**

**Chair: Alexandra Pinto | FEUP**

Cidália Botelho | FEUP

Daniel Direito | FEUP

Helder Xavier Nunes | FEUP

Joana Vilas Boas | FEUP

Marta Barbosa | FEUP

Sara Ramos | FEUP

<b>Fractionation of acids, ketones and aldehydes from lignin oxidation broth with SP700 resin</b>	
E. Gomes, I. Mota and A. E. Rodrigues . . . . .	29
<b>Oxypropylation of lignocellulosic agro-industrial residues – a comparative study</b>	
J.A. Pinto, M.N. Belgacem, A.E. Rodrigues, and M.F. Barreiro . . . . .	31
<b>Removal of Cr(III) by using activated carbons produced from rice waste chars</b>	
D. Dias, M. Miguel, M. Bernardo, N. Lapa, I. Matos, I. Fonseca, F. Pinto . . . . .	33
<b>Effects of Gallic acid on Membrane Biophysical Properties: Relevance for Its Biophysical Effects</b>	
Stephanie Andrade, Joana A. Loureiro, Manuel A. N. Coelho and Maria do Carmo Pereira . . . . .	35
<b>Liposomes for temozolomide delivery</b>	
M. J. Ramalho, Joana A. Loureiro, M. A. N Coelho and M. C. Pereira . . . . .	37
<b>Novel low cost ceramic and zeolite-ceramic composite membranes for liquid phase separation applications</b>	
R. Vinoth Kumar and G. Pugazhenthii. . . . .	39
<b>MSW energetic valorisation: sustainability analysis of a Portuguese incineration plant</b>	
Ana Ramos, Rosa Aragão, Carlos Afonso Teixeira, Abel Rouboa . . . . .	41
<b>Evaluation of the parameters affecting the photocatalytic reduction of CO<sub>2</sub> over graphene-based composites</b>	
H.F.V. Fontes, A.M.T. Silva, J.L. Figueiredo, J.L. Faria, L.M. Pastrana-Martínez. . . . .	43
<b>Performance of a passive Direct Alcohol Fuel Cell</b>	
Catarina Moreira, Beatriz Braz, Vânia Oliveira, Alexandra Rodrigues Pinto . . . . .	45
<b>Separation of Hexane Isomers Using ZIF-8</b>	
Adriano Henrique, José A. C. Silva and Alírio E. Rodrigues . . . . .	47
<b>Optimizing the Separation of Nadolol Stereoisomers by SMB Chromatography using Chiralpak IA Chiral Stationary Phase</b>	
Rami S. Arafah, António E. Ribeiro, Alírio E. Rodrigues and Luís S. Pais . . . . .	49
<b>Soybean oil methanolysis catalyzed by highly active CaO obtained from waste shells</b>	
R. Risso, P. Ferraz, S. Meireles, I. Fonseca and J. Vital . . . . .	51
<b>New Footwear Materials Based on Polyurethane and Polyureas</b>	
I.P. Fernandes, M.J. Ferreira, M.R. Costa and M.F. Barreiro . . . . .	53

## Separation of Hexane Isomers Using ZIF-8

Adriano Henrique<sup>1,2\*</sup>, José A. C. Silva<sup>1,2</sup> and Alírio E. Rodrigues<sup>2</sup>

<sup>1</sup> School of Technology and Management, Polytechnic Institute of Bragança, Bragança, Portugal;

<sup>2</sup> Laboratory of Separation and Reaction Engineering, Chemical Engineering Dpt., Faculty of Engineering University of Porto, Porto, Portugal.

\*[adriano\\_henrique@ipb.pt](mailto:adriano_henrique@ipb.pt)

**Keywords:** Hexane isomers, MOF ZIF-8, Multicomponent sorption, Breakthrough curves.

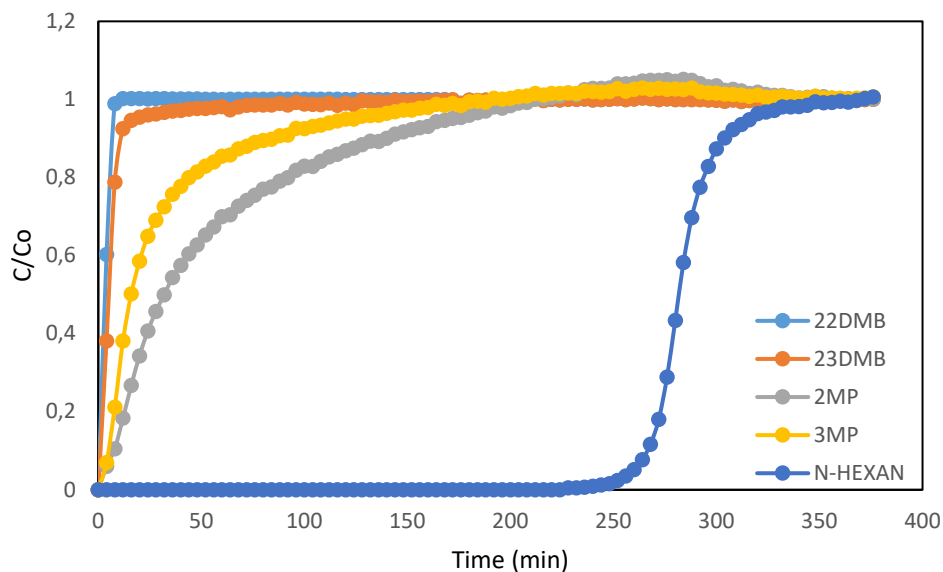
An important process in petrochemical industry is the octane upgrading of gasoline by the separation of paraffin isomers in the range C5/C6. The gasoline obtained from crude oil has a high fraction of linear and monobranched alkanes, which must be converted into isomers with high degree of ramification to improve the research octane number (RON) (Ferreira et al. 2013).

The RON is one of the parameters of gasoline quality and as higher its value, better is the combustion, reducing the tendency of a rapid and inefficient detonation of the hydrocarbons. In other words, the combustion occurs like a smooth explosion, improving the performance of the motor (Mendes et al. 2014).

The separation of n/iso-paraffins is actually realized by the Total Isomerization Process (TIP), which consist in performing the isomerization of normal paraffins, with low levels of RON to mono or di-branched isomers, and then, the paraffins with a high octane degree are separated from the others (Peralta et al. 2012). The research octane number increase as the branching degree of the paraffin increases.

In this way, the objective of this work is to study the separation of hexane isomers using a Metal Organic Framework (MOF) *i.e.* ZIF-8 (Zeolitic Imidazolate Framework) to improve the octane rating of gasoline in TIP processes. The MOF ZIF-8 shows chemical and thermal robustness and its structure consist of a cubic arrangement with 8 sodalite cages in the corner (Park et al. 2006).

In this work, several studies of the adsorption of hexane isomers on ZIF-8 were performed, with an equimolar mixture of: n-hexane (n-HEX), 2,2-dimethylbutane (22DMB), 2,3-dimethylbutane (23DMB), 3-methylpentane (3MP) and 2-methylpentane. During those experiments the temperatures and hydrocarbon pressure covers temperatures 373, 423 and 473 K and pressure range 2-10 kPa. Figure 1 shows a typical breakthrough curves for the C6 isomers at hydrocarbon pressure 5 kPa and temperature at 373 K.



**Figure 1.** Experimental breakthrough curve of an equimolar mixture of hexane isomers n-HEX/22DMB/23DMB/3MP/2MP at 373 K and hydrocarbon pressure at 5 kPa.

Figure 1 show that ZIF-8 is capable to perform the kinetic separation of hexane isomers in different classes, where the sorption hierarchy is: nHEX>>>2MP>3MP>>23DMB>22DMB. It is also being developed a numerical package using the Method of Lines (MOL) (Schuesser and Griffiths 2009) in MATLAB code to simulate the breakthrough-curves experiments.

From this work, it can be concluded that ZIF-8 can be an efficient separator of hexane isomers in classes: linear>monobranched>dibranched paraffins, with a high impact in the upgrading of actual TIP processes in petrochemical industry.

## References

- Ferreira, A. F. P., M. C. Mittelmeijer-Hazeleger, M. A. Granato, V. F. D. Martins, A. E. Rodrigues, G. Rothenberg. 2013. "Sieving Di-Branched from Mono-Branched and Linear Alkanes Using ZIF 8: Experimental Proof and Theoretical Explanation." *Phys. Chem. Chem. Phys.* 15 (22): 8795–804. Accessed 27 Feb, 2017. DOI: 10.1039/C3CP44381G.
- Mendes, P.A.P., A.E. Rodrigues, P. Horcajada, C. Serre, J.A.C. Silva. 2014. "Single and multicomponent adsorption of hexane isomers in the microporous ZIF-8." *Micropor. Mesopor. Mater.* 194: 146–156. Accessed 27 Feb, 2017. DOI: 10.1016/j.micromeso.2014.04.009.
- Park, K.S., Z. Ni, A.P. Côte, J.Y. Choi, R. Huang, F.J. Uribe-Romo, H.K. Chae, M. O'Keeffe, O.M. Yaghi. 2006. "Exceptional chemical and thermal stability of zeolitic imidazolate frameworks." *PNAS* 103 (27):10186–10191. Accessed 27 Feb, 2017. DOI: 10.1073/pnas.0602439103.
- Peralta, D., G. Chaplais, A. Simon-Masseron, K. Barthelet, G. D. Pirngruber. 2012. "Separation of C6 Paraffins Using Zeolitic Imidazolate Frameworks: Comparison with Zeolite 5A." *Ind. Eng. Chem. Res.* 51: 4692-4702. Accessed 27 Feb, 2017. DOI: 10.1021/ie202995g.
- Schuesser, W. E. and G. W Griffiths. 2009. *A Compendium of Partial Differential Equation Models. Method of Lines Analysis with Matlab.* Cambridge: Cambridge University Press.