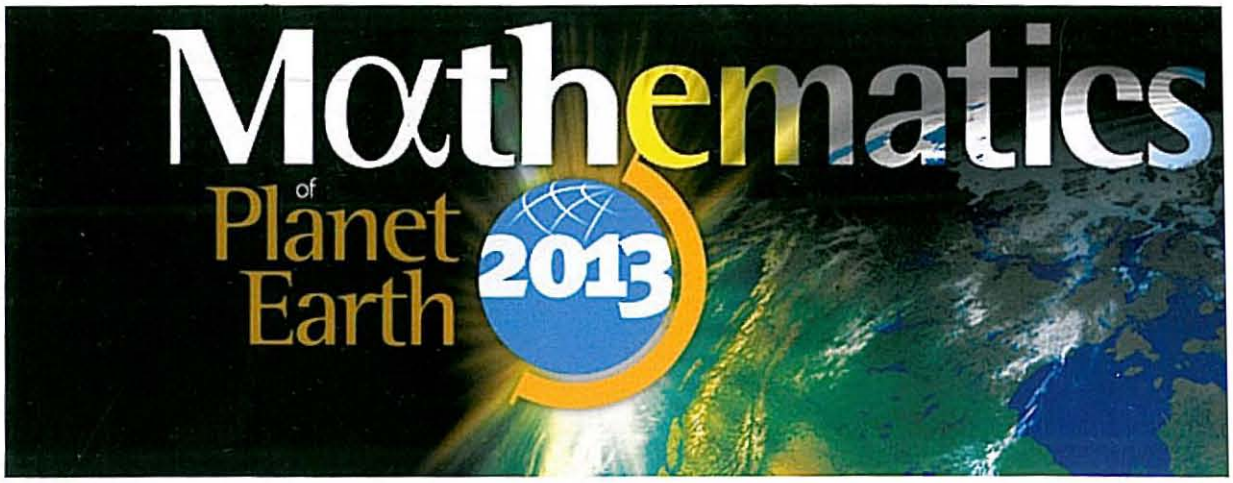

MECC 2013 - International Conference and Advanced School Planet Earth Mathematics of Energy and Climate Change

21-28 March 2013

Calouste Gulbenkian Foundation (FCG) and Faculdade de Ciências, Universidade Lisboa (FCUL)

Lisboa, Portugal

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Porous Solids for Biogas Upgrading and CO_2 Sequestration

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The reduction of CO_2 and CH_4 emissions to atmosphere is a matter of great concern nowadays since both gases can contribute significantly to the so-called greenhouse effect that describes the trapping of heat near earth´s surface by gases in the atmosphere. At the same time CO_2/CH_4 separations are of interest in treating gas streams like landfill gas, biogas and coal-bed methane. Accordingly, there is a need to investigate on this topic and that can be done with improved efficient technologies to separate or remove CO_2 and CH_4 from exhaust gases. Two recent reviews discuss this matter with great detail concerning the use of adsorbents (porous solids) based technologies to handle CO_2 capture and CO_2/CH_4 separations [1, 2]. Biogas is mainly composed by CH_4 (60 to 70%) and CO_2 (30 to 40%) and to obtain a high energy content CO_2 needs to be separated from CH_4. For this purpose a variety of solid physical adsorbents have been considered including molecular sieve zeolites and a new class of adsorbents named Metal-Organic Frameworks (MOFs). The technology for biogas upgrading using adsorbents is called Pressure Swing Adsorption (PSA). With this technique, carbon dioxide is separated from the biogas by adsorption under elevated pressure. The adsorbing material, is regenerated by a sequential decrease in pressure before the column is reloaded again, hence the name of the technique. In this work, we will present sorption equilibrium, kinetic and fixed bed data of CO_2, CH_4 in MOF-508b and zeolite 13X at 303, 323 and 343 K and partial pressures up to 4.5 bar. These data are fitted with appropriate isotherm models. At the same time single, binary and ternary breakthrough curves were measured to provide required data to develop and validate a mathematical model based on the LDF approximation for the mass transfer, which could be used in the implementation (simulation) of a cyclic adsorption processes (PSA) for the purification of biogas and CO2 sequestration.

[1] G. Férey, C. Serre. T. Devic, G. Maurin, H. Jobic, P. L. Llewellin, G. Weireld, A. Vimont, M. Daturi, J. S. Chang, Why hybrid solids capture greenhouse gases?, *Chem. Soc Rev.* 40 (2011) 550-562.

[2] D. M. D'Alessandro, B. Smit, Jeffrey R. Long, Carbon Dioxide Capture: Prospects for New Materials,*Angew. Chem. Int. Ed.* 49 (2010) 6058 - 6082.

Modelling and simulation of biodiesel production processes

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One can state that the application of the scientific method generally implies the construction of some kind of model which allows an easier way of dealing with and interpreting the complexity of the physical world. On the other hand, for millennia the mathematical language has proven to be an ideal code for the creation of these physical models of reality. Thus, much of the scientific process may encompass the tasks of mathematical representing the physical data (modelling), and then solving the obtained mathematical models (simulation) in various conditions. Here, we follow this two step process in order to study specific systems regarding chemical industrial processes for the production of biodiesel. Biodiesel is an alternative fuel to the conventional petrochemical fuels, and can be used as a total or partial substitute of petrodiesel in compression-ignition internal combustion