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Porous Solids for Biogas Upgrading and CO_2 Sequestration

José A. C. Silva [1,2,*], Alírio E. Rodrigues [2]

[1] Escola Superior de Tecnologia e Gestão, Instituto Politécnico de Bragança, Apartado 1134, 5301-857 Bragança, Portugal

[2] Laboratory of Separation and Reaction Engineering, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua do Dr. Roberto Frias, Portugal

*jsilva@ipb.pt

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

Marisa Novais [1], Paulo Tristão [1], Helder Gomes [1], Paulo Brito [1,2,*]

[1] Department of Chemical and Biological Technology, School of Technology and Management, Polytechnic Institute of Bragança, Campus de Santa Apolónia, PO Box 1134, 5301-857 Bragança - Portugal

[2] CIEPQPF, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Pólo II, Rua Sílvio Lima, 3030-790 Coimbra - Portugal

*paulo@ipb.pt

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 engines. It consists in a mix of alkylic esters usually synthesized by a transesterification reaction of triglycerides present in natural oils or fats, from vegetable or animal sources. We model and simulate biodiesel base-catalysed transesterification production processes in steady-state mode, using the simulation package UNISIM Design. This is a high level computational application that includes a user-friendly graphical interface which permits the building of industrial flowsheets through the connection of suitable unit operations, since it already comprises steady-state and evolutive general models for the most common industrial processes and the respective energy and mass connective streams. Hence, we present a simulation study including the synthesis, the biodiesel purification and the glycerol recovery processes, in order to prove the package suitability for mathematical representing these systems [1].

[1] Novais, M., Tristão, P.; *Simulação e optimização de processos de produção de biodiesel através do UNISIM DESIGN*, Renewable Energies Engineering Project, ESTiG/IPB, 2012.

Processing Renewable Energy for a Sustainable Planet

Vicente Leite
Escola Superior de Tecnologia e Gestão, Instituto Politécnico de Bragança, Apartado 1134, 5301-857 Braganą, Portugal
avtl@ipb.pt

Nowadays, and in the next decades, the number of systems based on electricity will grow up, and the consumption of electrical energy will strongly increase. Indeed, it is expected that more than 60% of all energy consumption will be converted and used as electricity [1]. This is the reality of developed and developing countries where there is an additional and urgent need of reducing CO_2. On the other hand, if we look at the planet as a whole, we find that there are extreme inequalities in access to electrical energy. Indeed, it is estimated that 1.4 billion people are living without electricity and according to the Organization for Economic Cooperation and Development (OECD), the electrification rate in Africa, in 2008, was 40% and less than 80% in the world. Consequently, it is mandatory to change from conventional to renewable energy sources and, on the other hand, promote the access to electricity for a huge part of the planet. In this way, we are witnessing a wide-spread integration of renewable sources in distribution networks and their dissemination in standalone systems, all over the world, either in small houses or islands and isolated regions. In fact, the electrical power technology is changing rapidly with the integration of a large number of dispersed generation units based on renewable and non-renewable sources are being installed everywhere [1, 2]. In this context, a powerful and flexible technology is needed, at reasonable prices, in a big part of the world aiming to promote the access to electricity. On the other hand, in developed regions, the efficiency of the technology used in power generation, transmission/distribution and end-user equipment has to be continuously improved and suitably designed for every application. In all cases, the gross electricity, as it is produced by different renewable sources, needs to be processed and integrated in order to be available in a suitable form for the transmission and the end-user. The Power Electronics, being the technology of efficient conversion of electric power, plays an important role in the above-mentioned scenario [1]. This paper describes how this technology, supported by advanced control algorithms, is enabling the access to energy to many people all over the world in a sustainable way, and describes the change from the traditional centralised power systems to a new paradigm, where more and more dispersed generation units based on renewable sources are being integrated in the power systems. The paper also describes how the electricity generated by different renewable sources can be integrated and processed in the context of a remote sustainable house, or in a developed power system, with the same quality of the electricity. Thus, even under a scenario of increasing consumption and growing access to the electricity by many people, it is possible to think of a more sustainable world, from a small house to the entire planet.