Intelligent Design of Nanoporous Sorbents (INDENS)

Proposal number : **005503**

Duration of Project : **48 months**

Contractors and places of implement of contract

Partner Legal entity	Acronym	Established in
Co-ordinator		
1a Centre National de la Recherche Scientifique	**CNRS / MADIREL**	**Marseille, France**
Other contractors		
1.b Centre National de la Recherche Scientifique, Délégation Régionale 07	**CNRSD - R07**	**Lyon, France**
2. The University of Edinburgh	**UEDIN**	**Edinburgh, UK**
3. J. Heyrovský Institute of Physical Chemistry	**JHI**	**Prague, Czech Republic**
4. The University of St. Andrews	**USTAN**	**St Andrews, UK**
5. National Technical University of Athens	**N.T.U.A.**	**Athens, Greece**
6. Universität Leipzig	**UNILEP**	**Leipzig, Germany**
7. SINTEF	**SINTEF**	**Oslo, Norway**
8. Institut Français du Pétrole	**IFP**	**Rueil-Malmaison, France**

Project Overview

Overall objectives

A number of applications use adsorption phenomena in nanoporous materials such as zeolites and metalaluminophosphate zeotypes. Major applications of such materials can be found in the domains of catalysis and ion-exchange as well as in selective adsorption and separation. In many cases, the materials used in a specific application have been found by trial and error or by systematic screening (combinational chemistry). Both of these approaches are essentially experimental and use empirical methods to explore a general class of materials. No prediction tools have been successfully used with respect to a given application.

The only simulation methods that have been dealt with up to now have been purely fundamental: either to randomly piece together secondary building units or to predict structures that arise during the synthesis after the use of a given organic template molecule. The increased power of computers and simulation methods means that it is becoming possible to benefit from computer aided tools such as Monte Carlo and Molecular Dynamics methods to predict the gas/solid behaviour and thus of the intrinsic physical and chemical properties required of the nanomaterial. This does not eliminate, however, an experimental validation. The present RTN project aims to investigate and INtelligently DEsign NanoporouS media most adapted for the storage/separation of specific gas molecules.

The aim of the present Marie-Curie training project is to form both Early Stage Researchers and Experienced Researchers in the dual fields of experiment and simulation with respect to given applications in the field of storage and separation of gases within nanoporous media. This project is perfectly relevant to the specific program structuring the European Research Area with Human

Resources and Mobility and more particularly with the Thematic Area 3 priority dedicated to Nanotechnologies and Nanosciences. The Research Training Network project aims to design the zeolite and zeotype materials, to predict their adsorption properties in industrial applications with respect to specific molecules and to experimentally evaluate their performance by measurements of pure gas / mixture adsorption and diffusion. Initial work will focus on the following gases:

- Carbon dioxide
- Methane
- Carbon monoxide
- Hydrogen

Whilst a large part of this project will be devoted to fundamental research, the role of the industrial partners and external consultants will be crucial in order to validate the choice of materials and to apply these materials under test conditions.

Overall approach and methodology

This work will combine modelling and experimental approaches by involving experts in the field of synthesis and experimental characterisation (adsorption, structure, diffusion), coupled with specialists in charge of the simulation of the synthesis process as well as the various properties of the nanoporous materials investigated. Each group is world leader in their respective field. The early stage and experienced researchers recruited under this project will be involved both in modelling and experimental studies within the different groups assembled in this network.

The scientific originality of this project will be thus the development of a tool which, starting from problems related to energy and environmental areas, is able to predict the structure and chemical composition of a given corresponding zeolite or zeotype. Building on this, specific synthesis routes will be developed to prepare such samples. The microscopic and macroscopic properties of these samples will be confronted with their performance in industrial tests. In this respect, this project is unique and ambitious.