EFCE Spotlight Talks

Working Party on Thermodynamics and Transport Properties

3 December

13:30 • 15:00 CET

Thermodynamic tools for CO2 capture

Energy efficient carbon dioxide capture has become one of the major industrial challenges of the coming decade. Today, the energy intensive absorption with amine solvents is the only proven solution. Yet other technologies are emerging, for which thermodynamic tools are being developed. This webinar will provide insight in these new technologies.

PROGRAM

Membranes for CO2 capture: thermodynamic aspects
Prof. Maria Grazia De Angelis, U. of Bologna (Italy)

Membrane separations appear as an economic and sustainable alternative to liquid-based processes in the removal of CO2 from gaseous streams in many industrial cases. In membrane processes, a leading role is played by the membrane material performance and its response to pressure, temperature, gas mixture composition and presence of impurities.
In the quest for the "Holy Grail" of membrane materials for CO2 capture, it is important to use accurate thermodynamic and transport models which can simulate the material behavior in a wide range of conditions, so to select the optimal polymeric membrane and enable an accurate design of the process.
In this webinar we will introduce and review the most advanced theoretical tools to simulate the membrane performance, in terms of selectivity and permeability, in realistic multicomponent conditions, taking the process of CO2 removal from natural gas and biogas as a case study. In particular, the polymeric membrane performance, that follows the solution-diffusion mechanism, can be predicted with equilibrium and non-equilibrium models for solubility based on equations of state like the SAFT and PC-SAFT ones, coupled to free-volume based models for diffusion.

Thermodynamic approach of demixing solvents
Dr. Pascal Mougin, IFP Energies nouvelles (France)

In the context of post-combustion CO2 capture, the search for new solvents is a very active path of research with the aim of reducing the energy cost of the capture process. This separation is based on the principle of a basic solvent that absorbs the acid gas and is recycled at high temperature and this last operation gives the cost of the process. A recent innovation proposed by IFPEN is to use a demixing solvent. After the CO2 absorption stage, the charged solvent is heated which leads to a liquid-liquid phase separation and thus it is possible to regenerate only the solvent rich in acid gas which reduces the energy cost of regeneration.
A large part of the data necessary for the dimensioning of the process concerns thermodynamic data: phase equilibrium, enthalpies and volumetric properties. Obtaining such data requires the use of different equipment to obtain these experimental data and their modeling uses reactive equilibria combining physical phase equilibrium and chemical reactions in the liquid phase. Reactive equilibria are generally represented by activity approaches dedicated to electrolytes: Debye-Hückel, Deshmukh-Mather, e-NRTL... and the enthalpic aspects are derived from Gibbs-Helmholtz equations.
In this webinar, we will present the experimental means necessary for the development of simulation tools and will discuss the development of such models to provide process tools.

registration

Contact:
martine.poux@toulouse-inp.fr
jean-charles.de-hemptinne@ifpen.fr