Research Topic for the ParisTech/CSC PhD Program

Field (cf. List of fields below): Chemistry, Physical Chemistry and Chemical Engineering

Subfield: (Applied Physics, Chemistry, Mathematics, Mech. Eng. etc…). Energy and environment. CO2 capture, NOx capture.

Title: Modelling the thermodynamic properties of electrolyte systems. Application to the simulation of novel flue gas treatment processes

ParisTech School: ENSTA ParisTech

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Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

Flue gas treatment is the process used to reduce the amount of pollutants emitted from the combustion of fossil fuels (coal, natural gases, wood, …). It is crucial for the reduction of pollution from coal / diesel power plants. Flue gases contain a significant amount of nitrogen oxides, CO2, and sulfuric compounds (H2S, SO2) that affect the quality of air. These compounds can be captured by using different processes such as scrubbing columns. The chemicals used in these columns to capture pollutants are mainly electrolyte aqueous solutions. The flue gas treatment requires a significant amount of energy (heat) during the desorption process of the pollutants. In order to assess the amount of energy needed and the efficiency of the process, one must perform a reliable design by using a process simulation software based on an accurate thermodynamic model. Such a model should take into account all chemical reactions and ionic species. The aim of this project is to develop a reliable thermodynamic model for electrolyte solutions and apply it for the simulation of novel gas treatment processes.

Required background of the student: (Which should be the main field of study of the applicant before applying)

The student should have a master degree in chemistry, physics, energy, or chemical engineering. He/she must have a good background in chemistry, maths and programming.

A list of 5(max.) representative publications of the group: (Related to the research topic)

[1] A. G. Perez, C. Coquelet, P. Paricaud, A. Chapoy, Fluid Phase Equilib, 440, 19-35 (2017).
[2] P. Babu, P. Paricaud, P. Linga, Fluid Phase Equilib., 413, 80-85 (2016).
[3] A. Fukumoto, P. Paricaud, D. Dalmazzone, W. Bouchafaa, T.T.S. Ho, W. Fürst, J. Chem. Eng. Data, 59, 3193-3204 (2014)