Ph.D. thesis position
Chemical-engineering thermodynamics

■ General information

Topics:	Chemical-engineering thermodynamics.
Title:	**Quest for the thermodynamic Holy Grail:** Development of a **universal thermodynamic model** for phase-behaviour and energetic property description having the following features: (1) **capable of accurately describing mixtures in which hydrogen bonds occur** (2) **predictive** (model inputs are molecular structures) and (3) **applicable to any non-electrolyte mixture involved in any chemical-engineering process (i.e., ready for industrialization)**
Funding:	TOTAL Grant from the TOTAL company. Possibility to supplement the salary by teaching (only for people speaking French). ***Basic salary:*** 1800 € / month (before taxes).
Dates:	October 2018 - September 2021.
Place:	Team ThermE (thermodynamics and energy), *of the* LRGP (Laboratory for Reactions and Chemical Engineering) – University of Lorraine, Nancy, France.
Ph.D. supervisors:	**Jean-Noël Jaubert**, professor. ✉ `jean-noel.jaubert@univ-lorraine.fr` ☎ (+33)3.72.74.37.70 **Romain Privat**, associate professor. ✉ `romain.privat@univ-lorraine.fr` ☎ (+33)3.72.74.37.73

■ Ideal candidate's skills

- Good knowledge in chemical engineering, thermodynamics and mathematics (numerical methods)
- Problem solving orientation
- Knowledge of a computer-programing language (ForTran ideally)
- Communication skills (in English)

■ Application

To apply, send your CV and a motivation letter to Jean-Noël Jaubert and Romain Privat.

■ Scientific content

Today, the synthesis design and optimization of the processes are carried out with the help of process simulators (ProSim, PRO/II, ASPEN ...). It is well admitted that the accuracy of the simulated results mainly depends on the quality of the thermodynamic model. In most cases, the phase behavior of multi-component systems for which nearly no data are available has to be known. In addition, energetic properties (enthalpy, entropy, exergy, heat capacity ...) are systematically required for calculating energy and entropy balances and thus, to perform exergy analysis.

Phase behaviours and thermodynamic properties can obviously be measured, but measurements are very time consuming. This is why modern process design requires models:

- capable of predicting the equilibrium properties without the preliminary use of experimental data,
- yielding accurate results in both the sub- and super-critical regions,
- ensuring an acceptable level of accuracy in energy, entropy and exergy balances.

Simultaneous fulfillment of these requirements is a very difficult and challenging task for a thermodynamic model.

Objectives of the thesis:

Our research group is specialized in the development and parameterization of equations of state (EoS). For many years, we are working conjointly on two EoS classes: the cubic models (issued from Van der Waals' seminal work) and the SAFT-type models (SAFT stands for "Statistical Associating Fluid Theory").

Numerous successes were obtained in the past years by our team including the description of pure-component properties with an unprecedented accuracy and the development of efficient predictive methods making it possible to guesstimate phase behaviours and energetic properties of complex non-associating mixtures (i.e., mixtures that are free of hydrogen bonds).

Although more and more addressed in the open literature, the prediction of thermodynamic properties in associating mixtures remains a challenge.

The ultimate goal of this Ph.D. thesis is to develop two efficient predictive thermodynamic models (a SAFT-type one and a cubic-type one), capable of accurately describing associating and non-associating mixtures and applicable to large range of molecular species and related mixtures.

Methods: Efficient SAFT and cubic models for non-associating mixtures have been recently developed by our team.

To make these models applicable to associating mixtures, a specific term accounting for associating phenomena must be added.

The expression of this additional term depends on:

- a so-called association scheme (i.e., the number of H-bond donor/acceptor sites present on each molecule),
- association parameters.

The Ph.D. candidate will be asked first to develop methods for choosing an appropriate association scheme and determining the corresponding association parameters.

Secondly, he will address their prediction.