Ph.D. thesis position
Chemical-engineering thermodynamics

■ General information

Topics: Chemical-engineering thermodynamics.

Title: **Novel modelling ways for describing fluids:**
This work is devoted to develop and benchmark **2 new types of models** for pure species and mixtures based on: (1) an extended version of the corresponding-state law and (2) a nearly-unexplored way to improve predictions of cubic equations of state.
This challenge is likely to highlight new horizons for thermodynamic modelling; it is ideal for students who are ready to commit themselves 100% and participate in an ambitious project.

Funding: Scholarship from the GTT company
https://www.gtt.fr/en

Gross salary: 35 000 € / year (approximately).

Dates: October 2021 - September 2024.

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**, full 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
- High work capacity
- Knowledge of a computer-programing language (ForTran ideally)
- Communication skills (in English or in French)

Note that the thesis work will be purely theoretical and numerical (no experimental work).

■ Application

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

■ Scientific content

Our team:
Our research group is specialized in the development and parameterization of equations of state. 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 behaviors and energetic properties of complex non-associating mixtures (i.e., mixtures that are free of hydrogen bonds). Among these, let us cite: the PPR78 and E-PPR78 models, the PR2SRK model, the I-PC-SAFT model, all available in commercial simulation software and regularly used by the scientific community.

Objectives of the thesis:
However, despite intensive efforts, progress remains to be made in fluid modeling. Regardless of the approach chosen (SAFT or cubic), equations of state are still struggling to simultaneously reproduce phase equilibria, volumetric and energetic properties of fluids, in particular when approaching the critical region.
While 99.99 % of current equations of state are classically derived from well founded SAFT or cubic theories, some unexplored or nearly-unexplored ways deserve interest and could have the potential to move the lines. In this thesis, two types of unusual models will be studied:

- A model derived from an extended version of the corresponding-state law (inspired from the works by Leland et al. and Ely; for more details, see e.g., Ely J.F. (1990) A Predictive, Exact Shape Factor Extended Corresponding States Model for Mixtures. In: Fast R.W. (eds) Advances in Cryogenic Engineering. Advances in Cryogenic Engineering, vol 35. Springer, Boston, MA),
- A cubic-type model involving a temperature-dependent function in the polynomial in volume of the attractive term.

In both cases, our preliminary calculations show very promising results that need to be confirmed and boosted through the thesis work.

Collaboration: the development of the corresponding-law equation of state will be performed in collaboration with Paul M. Mathias, world-renowned expert in thermodynamic modelling.