

## **PhD position in the heart of Europe - Nancy, France**

Laboratoire Réactions et Génie des Procédés (Laboratory of Reactions and Process Engineering)

CNRS-Université de Lorraine (CNRS UMR 7274-University of Lorraine)

LRGP-ENSIC, 1 rue Grandville, BP 20451, 54001 Nancy, France

### **Modeling of chemical and biochemical processes using advanced phenomenological and data-driven techniques**

#### **General context**

Modeling of chemical and biochemical systems has come a long way over the last decades, with the development of powerful numerical techniques that exploit to the maximum the ever-growing computer power and our increasing understanding of the mechanisms governing these systems. At the same time, a parallel breakthrough is observed on the field of machine learning, with the development of deeper artificial neural networks (ANN), capable of better "understanding" and predicting the behavior of physical systems. Unfortunately, the implementation of such approaches to problems in the area of chemical and biochemical engineering remains rather limited.

A reason for this is their demand for elevated simulation times and large data sets, the latter often posing a significant limitation since the generation of data of physicochemical systems is often time-consuming and costly. In addition, despite their predicting capabilities, neural networks are yet another type of multi-parametric models, a fact that creates a bottleneck in any modeling approach. Besides ANNs, a plethora of alternative data-driven techniques are commonly employed in the areas of cognitive sciences, robotics and automation, that could eventually be proven well-suited and extremely efficient to problems in the process engineering domain. The so-called non-parametric models offer a promising alternative, with characteristics quite different to those of ANNs.

#### **Objectives of the PhD**

The objective of this work will be to investigate the implementation of various modeling approaches to different physicochemical systems. The applications will be primarily related to polymer synthesis and/or modification systems, already under study in the framework of previous or ongoing research studies of the group. In this respect, some data are/will be readily available. Existing modeling developments might also exist for some of them.

The work of the successful candidate will be to investigate possible improvements and/or new developments on the modeling of these systems, with a principal focus on data-driven techniques. It is expected that, after an initial period of intensive literature study, (s)he will be in position to propose and implement the appropriate modeling approaches according to the nature of the different applications and the characteristics of each technique. Although the work will be primarily theoretical, on the development of mathematical models and the execution of computer simulations, it is not excluded that some limited experimental work might be required to eventually generate additional data.

#### **Indicative relative literature**

*Meimaroglou D. and Kiparissides C., Ind. Eng. Chem. Res., 2014, 53, 8963–8979*

*Pirdashti M., Curteanu S., Kamangar M. H., Hashim M. H. and Khatami M. A., Rev. Chem. Eng., 2013, 29, 205-234*

## **Requirements**

We are looking for a highly-motivated PhD candidate, with basic understanding of chemical or process engineering, with a proven talent for computer programming and simulation. More specifically:

## **Prerequisites**

- Good knowledge of Matlab or any other similar package (e.g., Scilab).
- Excellent written and spoken English.
- Basic knowledge of polymer science.
- Basic knowledge of statistics.
- Motivation to carry out a major part of the PhD in developing and running PC programs.

## **Additional appreciated skills**

- Master degree on related fields (e.g., polymer science, data treatment, etc.).
- Knowledge of any other programming language or software (e.g., Fortran, VBA, Python).
- Any level of French and/or willingness to improve it.
- Organizational skills and capacity to adapt and evolve his/her learning methodology.

**Monthly salary:** ~1760 € gross (for 3 years)

**Starting date:** October 2020

**Deadline for applications:** April 30, 2020

## **Application Procedure**

All applications are to be sent directly to the following address: ***name@domain***, where: ***name:*** dimitrios.meimaroglou and ***domain:*** univ-lorraine.fr (please use the following e-mail subject: "Application for PhD on modeling").

Applications must include a CV and a short motivation letter. Any additional document that might support your application (e.g., transcript of grades, recommendation letters, etc.) are welcome. Do not send copies of your degrees at this stage!

After an initial shortlisting stage of the applications, selected candidates will be called to a remote interview. The final candidate will need to constitute an online application on the relevant university website and provide additional documents for the administrative enrollment (e.g., ID card, insurance, etc.).

For more information on the administrative procedures, please visit:

<http://doctorat.univ-lorraine.fr/en/doctoral-studies-UL/doctoral-system>

<http://doctorat.univ-lorraine.fr/en/doctoral-schools/simppe/presentation>