



Advanced modelling of complex reaction network : from feedstock molecular reconstructing to single events kinetics network generation

Date : 22/05/2013

IFP Energies nouvelles

Division : Process Design and Modeling Division

Offer Details

Duration: 12 months

Starting Date: September 2013

Salary (gross) : 42 k€/year

Location: Solaize (near Lyon), France

Missions

The construction of kinetic models is a key step in the development of refining processes to predict the performances, optimize the process operation and design reactor and process configurations. For refining conversion process of heavy oils, the current demand for models is particularly focused towards the development of detailed predictive models that are able to account for significant changes in process operation. Hence, they need to handle large range of operating conditions and variety of feedstocks.

Kinetic modelling based on the single-event theory meets these requirements, since it allows detailed prediction of the composition, and hence the yield structure from the reactors. This methodology consists in constructing a reaction network which, although exhaustive, is described by a limited number of independent kinetic parameters. The application of this technique to complex process is a challenge according to the complexity of the feed and reaction network.

The overall objectives of the postdoctoral position are :

- To complete, improve, merge and test advanced models developed by several PhD students^{1,2} (using stochastic reconstruction, single event methodology...)
- Apply the modelling approach to industrial conversion refining process and validate it by comparing experimental data to simulation results.
- To use this new simulator in order to propose innovative process configurations
- To validate the proposed methodology in order to use it on another chemical process.

¹Guillaume et al. (2011), Single Event Kinetic Modelling without Explicit Generation of Large Networks: Application to Hydrocracking of Long Paraffins, *Oil Gas Sci. Technol.*, Vol 66, No 3

²Charron et al. (2011), Kinetic Modeling of Vacuum Gas Oil Hydrotreatment using a Molecular Reconstruction Approach, *Oil Gas Sci. Technol.*, Vol. 66, No 3

Formation

Candidates must hold a PhD in Chemical/Process Engineering, Mathematics or equivalent and a good understanding of mathematical/computational, model-based techniques for optimisation.

Canidate's profile

Experience in using computational tools such as Fortran, C++, Java and MATLAB, or equivalent modelling and optimisation tools, is required.

Knowledge of refining area is an advantage but not compulsory.

The post requires autonomy, rigor, powers of analysis and synthesis, and at the same time of creativity, as well as strong technical skills in computer science, kinetics and reaction engineering and modelling.

Contact : Benoit CELSE (benoit.celse@ifpen.fr) or Denis GUILLAUME (denis.guillaume@ifpen.fr)