



Post-doctoral Position: New methodology for identifying descriptors of bifunctional catalysts by kinetic approach and Machine Learning

If you wish to evolve in a challenging technical environment in the Energy Transition area, if you are an expert in Data Science and if you are autonomous and motivated to tackle a major technical issue in chemical engineering, this job is for you!

Job description

IFP Energies Nouvelles is a French public-sector research, innovation and training center active in the fields of energy, transport and the environment.

In order to ensure a reliable extrapolation of a chemical process, for instance to produce renewable fuels from biomass feedstocks, the reactor modeling is an essential step. However, a model is generally developed only after a new catalyst has been validated and the performance of a future catalyst cannot be predicted.

The objective of this post-doctoral position is to integrate catalyst descriptors into reactor performance predictive models, in order to accelerate the development phase of reactor models by integrating a priori information inherent to the catalyst, but also in order to drive the development of new catalysts by rationalizing the impact of physico-chemical properties of the catalysts on their performances at industrial reactor scale. The proposed field of application is the family of bi-functional catalysts, which will concern in the near future the processes of fuel production from the conversion of biomass or recycled waste and plastics.

The performance of chemical processes is mainly determined by the operational conditions (temperature, pressure, LHSV, load) which can obscure the impact of catalyst properties in a simple data analysis. The originality of this work is to use kinetic models to overcome this problem. By developing a bank of kinetic models for each catalyst formulation, the reactivity of the catalysts can be evaluated independently of the operational conditions. In this way, the machine learning approach can be fruitfully applied, having a raw data set to analyze the relationships between physical properties and catalyst performance, independent of variation in feedstock and process conditions.

The research work is expected to result in publications in scientific journals. The development is expected to be done in R or Python.

Qualifications

Application-interested candidates with a strong computational background are encouraged to apply. The required Skills and Experience are:

- Master in relevant field (Chemical Engineering, Data Mining/Data Science or Computer Science)
- Data science, parameter tuning, optimization, numerical analysis
- Programming languages: Python, R
- Proficiency in English
- Good listening skills, rigorous and pragmatic
- Good communication skills, oral and written

Location

IFP Energies nouvelles
BP3 - Rond point de l'échangeur de Solaize (15 km south of Lyon)
69360 Solaize. France

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Informations

Desired duration: 12 months
Desired period: 2021
Location: IFP Energies Nouvelles - Lyon
Application: Please send your application (CV, cover letter, Statement of Research Interests, References) to leo.violet@ifpen.fr

