Internship: Physics-Informed Machine Learning for catalytic hydrocracking process modeling

Laboratoire ERIC, Université Lyon 2,

In collaboration with IFPEN

1. Context

This internship take part of a collaboration between IFPEN (https://www.ifpenergiesnouvelles.fr), ERIC laboratory (https://eric.msh-lse.fr) and LabHC (https://laboratoirehubertcurien.univ-st-etienne.fr/), which aims to develop hybrid model for physicochemical processes.

IFPEN is a major player in the development of catalytic processes, primarily for the development of new generations of biofuels, for the chemical recycling of plastic and tire waste, and for reducing the environmental impact of oil refining. We are a leader in the development of reliable and robust reactor models required for the design and operation of industrial units. This work is essential for the ecological transition.

However, knowledge models, based on the theoretical laws of physics, do not always describe all the physicochemical phenomena involved, either because some are unknown or because the models must be simplified for reasons of cost and complexity.

2. Subject

The objective of this internship is to improve existing models, relying on hybrid modeling approaches or physics-informed machine learning, combining knowledge models and data-driven machine learning models. The advantage is that each can compensate for the disadvantages of the other. However, the scenario in which (i) physical theory only partially explains the observations and (ii) there is a shortage of data has been little explored in the literature to date. Several coupling strategies, adapted to the constraints and challenges of the application case, will therefore be developed and analyzed. They will be evaluated based on criteria of accuracy, extrapolation capacity, sensitivity to the volume and nature of the data, and complexity.

The application case will be the catalytic hydrocracking process, for which IFPEN has developed around ten catalysts, but whose performance cannot yet be predicted with a single, catalyst-independent model.

The internship will take place at the ERIC laboratory, with close interaction with IFPEN.

The internship may be extended by a thesis at IFPEN, part of a cluster of theses focusing on the development and analysis of hybrid modeling strategies.

3. Some references

1. Hao Z, Liu S, Zhang Y et al. Physics-Informed Machine Learning: A Survey on Problems, Methods and Applications (2023). arxiv.org/pdf/2211.08064v2.

2. Karniadakis GE, Kevrekidis IG, Lu L, Perdikaris P, Wang S, Yang L. Physics-informed machine learning. Nat Rev Phys 3(6), 422–440 (2021).

3. Bradley W, Kim J, Kilwein Z et al. Perspectives on the integration between first-principles and data-driven modeling. Computers & Chemical Engineering 166, 107898 (2022).

4. Internship conditions

Location: the intern will join the Data Mining & Decision team of the ERIC lab. (Campus Porte des Alpes, Bron), which is composed of 13 permanent researchers in statistics and computer science and about 15 Phd students.

Duration: 6 months, starting in March 2026 or earlier

Salary: approx. 30€ / day

Contact and supervision: julien.jacques@univ-lyon2.fr