

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 actor in the development of catalytic processes, mainly for the development of the 2nd-generation of biofuels, for the chemical recycling of plastic and tire waste, and for the reduction of 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. However, knowledge-based models, relying on theoretical laws of physics, do not always describe all the physicochemical phenomena involved, either because some are unknown, or because the models have to be simplified for cost or complexity considerations. This is typically the case for modeling the catalytic hydrocracking process, for which IFPEN has developed a dozen or so catalysts, but whose performance cannot yet be predicted with a single, catalyst-independent model.

2. Subject

The aim of this internship is to develop this unique catalyst-independent model, based on hybrid modeling approaches or physics-informed Machine Learning, combining knowledge models and data-based Machine Learning models. The idea is that each model should be able to compensate for the disadvantages of the other. Several coupling strategies, adapted to the constraints and challenges of the application case, will therefore be developed and analyzed. They will be evaluated according to criteria of accuracy, extrapolation capacity, sensitivity to data volume and nature, and complexity.

This internship might be followed by a PHD at IFPEN-Lyon in collaboration with the ERIC lab on the same subject.

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. A part of the internship will be done at IFPEN (Solaize).

Duration: 6 months, starting in March 2025

Salary: approx. 30€ / day

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