Artificial intelligence to guide the eco-design of chemicals and anticipate life-cycle environmental impacts

Do you want to employ your computer science and AI skills to help the environment? Do you wish to create new tools and methods, in support of agile eco-design of chemicals with a major industrial player? Can you imagine yourself contributing to more robust and complete assessments of future environmental impacts?

If so, this Ph.D. project might be for you!

The research challenge:

To design chemicals that are genuinely environmentally friendly, it is crucial to assess the many different types of environmental impacts that they can cause, both directly through their release and indirectly through their production and end-of-life treatment. Currently, reaching such a life-cycle perspective for even a small number of chemicals is time-consuming and costly. Extending such a life-cycle assessment (LCA) to the hundreds of chemical design candidates that are considered in the early stages of an eco-design process is simply infeasible. The goal of this project is to rely on artificial intelligence (AI) to quickly predict this missing LCA data for innovative chemicals based on their properties and that of their typical production processes.

Industrial Context:

TotalEnergies has a new climate ambition to become a Net Zero Emission Company for all its businesses by 2050. To support this effort, a new eco-design R&D team was created to develop more environmentally responsible products, esp. improved lubricants. This project will create a new, open-source tool to support this team with estimation of missing data, anticipation of future environmental impacts, and uncertainty analysis. These predictive models (*in silico* screening and *in silico de novo* design) will help the researchers to choose the ways of formulation with the least environmental impacts, especially those required for the European PEF methodology.

Academic Context:

This fully funded Ph.D will be hosted by the Chemical engineering department of Polytechnique Montreal, a world-class engineering school and a leader in numerical modelling. You will also join the CIRAIG research centre, a dynamic multidisciplinary team advancing the assessment and optimization of sustainable of production and consumption systems. The CIRAIG is internationally recognized for its solid scientific research and applied experience working in partnership with industry and governments. We strive for academic excellence performed in a dynamic and pleasant community characterized by collegial respect and academic freedom.

Candidate profile

We seek a candidate with an engineering, computer science, or natural science background. Scientific programming, IT skills, or AI competences are important assets. We seek a candidate with a vivid interest in sustainability research, although previous training in ecodesign or LCA is not necessary.

Equity, diversity and inclusion

We strongly welcome and encourage applications from racialized persons, visible minorities, women, Indigenous persons, persons with disabilities, ethnic minorities, and persons of minority sexual orientations and gender identities, as well as from all qualified candidates with the skills and knowledge to engage productively with diverse communities.

Key words

Life-Cycle Assessment (LCA), Eco-design, Data management, Artificial Intelligence, Predictive models, Machine learning, Green Chemistry

Timing

4 years, ideally from January 2023

Languages

- English
- French (optional)

Contacts:

Please send your CV, motivation letter, diplomas, and transcripts of records to :

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