Assistant Professorship of Sustainable Future Mobility
TUM School of Engineering and Design
Technical University of Munich

Fuel Design and Surrogate Modelling with Machine Learning

Position: Master thesis

Type: Computational and theoretical

Job Description

The fuel design concept focuses on developing reaction mechanisms for fuel oxidation and energy conversion, aiming for lower fuel consumption and minimal pollutant emissions. To model the complex behaviour of real fuels, which may contain hundreds of components, we use the surrogate fuel approach. Surrogates consist of a reduced number of representative molecules that collectively reproduce the physical and chemical properties of real fuel blends.

In this project, we aim to develop a numerical tool to automatize the construction of comprehensive surrogate fuels that accurately emulate fuel key properties, such as: Molecular class composition, Molecular weight range, Hydrogen-to-carbon ratio (H/C), Derived Cetane Number (DCN), Threshold Sooting Index (TSI), Viscosity, combustion enthalpy, energy density, Distillation characteristics and vapor-liquid equilibrium, Combustion behavior: ignition delay times, laminar flame speeds, species concentration profiles.

Your Tasks

- Design and develop a numerical tool in Python for the construction and optimization of the Input Formula for Surrogate (IFS)
- Integration of multiple calculation modules into an optimization loop
  Module I - Database of physical properties for individual hydrocarbons and carbon-free molecules for “green” fuel design
  Module 2 - Module for calculating additive properties
  Module 3 - Module for predicting boiling points and phase behaviour (e.g., two-phase diagrams)

Our Requirements

- Background in chemical engineering, mechanical engineering, physics, or related fields
- Programming skills in Python
- Interest in clean energy, combustion, or fuel design
- Motivation to work independently within a supportive team

Our Offer

- Hands-on experience with machine learning, numerical modelling, and chemical engineering
- Insight into advanced fuel research relevant to aviation, space, and marine applications
- Opportunity to contribute to cutting-edge sustainable fuel technology

Contact

If you have any questions or are interested in working with our team, please send your application to Dr. Nadezda Slavinskaya (nadja.slavinskaya@tum.de).