Direction Mobilité et Systèmes
Stage R10/2027/n° 15

Sustainable Aviation Fuels:
Database Development and Property Prediction using Machine Learning

Description:

Among the various ways to decarbonize the aviation sector, sustainable aviation fuels (SAF) remain the most promising short-term solution, as they aim to be "drop-in" fuels that require no or limited hardware modifications and can be blended with conventional jet fuels. Currently, SAF from different production pathways are allowed by a maximum incorporation rate of 10% to 50% into conventional kerosene. And 100% SAF is expected in the near future, as discussed by various certification organizations. However, this results in challenges in terms of physical and chemical properties that remain unclear and difficult to anticipate for SAF and their blends, as they introduce significant differences and increased variety in composition with respect to conventional jet fuels whose composition remains unchanged for more than 80 years. The challenges mainly originate from: (i) lack of data for the properties of these future fuels, (ii) out of validity range for some existing models designed for conventional fuels, and (iii) complexity in blending and formulation which requires better understandings on their mixing behaviors. Therefore, it is necessary and essential to build a comprehensive database and improve predictions on the physical and chemical properties of sustainable aviation fuels and their blends.

In this context, IFPEN is in a central position as we have expertise in both the production processes and the utilization with knowledge of fuel formulation. Following our previous developments of a fuel database with APIs and a user interface which empowers machine-learning models, we propose this internship to further enhance our activities on sustainable aviation fuels, with the following tasks:

- Fuel-property database development
  - Improvement of the database architecture, data quality, APIs, and UI to support the storage, management, visualization of fuel composition and property data, and implementation of models.
  - Integration, curation, and validation of experimental and literature data from various sources, with particular attention to data consistency, traceability, and usability for scientific applications.
- Property prediction using machine learning
  - Prediction of multi-dependency fuel properties from fuel composition or other physicochemical properties, for example temperature- and/or pressure-dependent properties.
  - Prediction of fuel families, blending components and fractions, and mixture properties from compositional and physicochemical information.
- (Optional) Exploration of advanced data-driven methodologies
  - Investigation of learning strategies for sparse and heterogeneous datasets while preserving data fidelity, and other topics including uncertainty quantification, active learning, and knowledge management.

Required Profile: Bac+4 or Bac+5 in Computer Science, Data Science, or related fields.

Proficiency in relational database, machine learning, and AI tools. Familiar with API, Web UI Design, GitLab, etc. Ability to code and write in English.

Keywords: Sustainable Aviation Fuels, Property Prediction, Relational Database, Machine Learning
Duration and Date: 5-6 months in 2027
Location: Rueil-Malmaison or Solaize. The student can choose according to his/her convenience.
Contact Persons for Application: boyang.xu@ifpen.fr, didier.grondin@ifpen.fr
Telephone: 01 47 52 71 15