

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

Description:

Among the various ways to decarbonize the aviation sector, sustainable aviation fuels (SAF) remain the most promising solution for the short term, as they aim to be “drop-in” fuels which require no or limited hardware modifications and can be blended in 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 on both the production processes and the utilization with knowledge on fuel formulation. We propose this internship to further enhance our activities on sustainable aviation fuels, with the following tasks and focus on database development.

- Design of the structure of a comprehensive relational database for fuel properties. Such well-designed structure aims to achieve the following features.
 - Breakdown design for fluid compositions (e.g., parent and child fluids) with capability to compute the decomposed composition at any level.
 - Flexible design for property dependency, i.e., a property can depend on an arbitrary number of other properties. Such design will be capable to store not only temperature- and pressure-dependent properties, but also more sophisticated data like IR spectra, GCxGC results, distillation curves, etc.
 - Capability for end users to not only add/edit values but also define new properties.
 - Storage of models with well-defined metadata and executable commands for automated computations.
- Filling of content of the database using various methods.
 - From data already available at IFPEN.
 - Automatic data retrieval from literature using AI and machine learning approaches.
 - Automatic property predictions using models defined in the database.
- Prediction of a selected property using machine learning methods.
 - Based on constructed database, explore the relationship of a selected property with compositional, other physiochemical properties, and/or spectra, using statistical learning methods best suited for the data features.

Required Profile: Bac+4 or Bac+5 in Computer Science

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 2026

Location: Rueil-Malmaison or Solaize. The student can choose according to his/her convenience.

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