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

# Model database creation for combustion of Sustainable Aviation Fuels

Type: Master Thesis
Content: Theoretical / Numerical
Possible start: As soon as possible

## Job Description

As the world moves towards technologies with lower carbon footprint, Sustainable Aviation Fuels (SAF) form an important constituent of existing fuels for aviation and are expected to play a major role in the near future. Understanding their impact on combustion processes and emissions requires a good knowledge of the chemical reactions involved in the combustion of these hydrocarbons. With this in view, our team is working towards building reduced kinetic schemes for surrogate fuels representative of various types of SAF. To do this, an in-depth understanding of the chemical kinetics of the constituent hydrocarbons for each type of SAF is required. This can be achieved by reproducing the experimentally measured chemical species concentrations in flames of various 0D/1D canonical configurations (shock tube measurements, laminar premixed flames, counterflow diffusion flames).

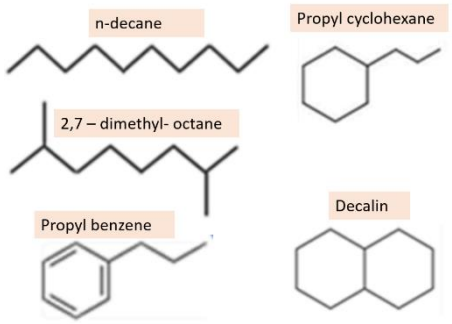

*Figure: Some hydrocarbon constituents of SAF*

A series of experimental datasets for different constituent hydrocarbons of SAF have been identified (for example: Figure above). The candidate is expected to perform simulations using computational packages for chemical kinetics and soot (Ex: CANTERA/FlameMaster) for each of these hydrocarbons. The intent is to create a database of models for various fuels for the said flame configurations, which can be then used to test reduced kinetic schemes to be developed in parallel in our team. In future, the database generated is intended to be used for the verification of detailed/reduced chemical kinetic schemes generated for surrogate fuels for SAF and for polycyclic aromatic hydrocarbons (PAH).

## Your Tasks

- Simulate canonical flame configurations using FlameMaster/CANTERA
- Model independent hydrocarbon constituents of SAF
- Compare species concentrations for each case and investigate trends and possible reasons for a match/mismatch
- Archive the database of the models

## Recommended Prior Knowledge

- Background in thermodynamics, numerical modeling
- Working in Linux/C/FORTRAN/Python or willing to learn
- Able to communicate in English
- Prior knowledge of combustion or chemical kinetics is an advantage but not essential

**Contact**: If you are interested in working in our team, please send your application together with a motivation and supporting documentation to Pavan Prakash Duvvuri (pavan.duvvuri@tum.de). If you have any questions, do not hesitate to contact us.