Aerodynamisches Institut und Lehrstuhl für Strömungslehre | RWTH AACHEN UNIVERSITY

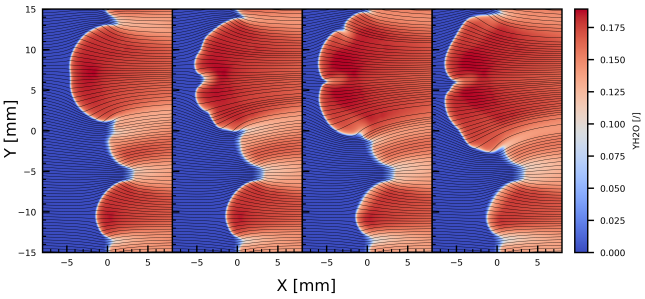
Master Thesis

Machine learning-based modeling of non-equilibrium chemical reaction rates for the computation of hydrogen-air flames

Hydrogen combustion is shaping to be an important component for the future of electricity grids based on renewable energies. Combustion simulations solve the mass, momentum and energy equations in addition to equations describing the reaction kinetics and transport of species. These additional equations are, in general, expensive to solve when compared to the non-reacting flow equations.

In order to reduce computational expense, some simplified alternatives exist, like skeletal reaction mechanisms or two-step chemistry. If one desires to use the complete, relevant reaction chain, tabulated chemistry or machine learning models are a good alternative and a good compromise between accuracy and efficiency. In this context, four types of machine learning algorithms are employed. The first algorithm maps each location in the high-dimensional flow domain to a low-dimensional subspace. With the second algorithm, representations in the low-dimensional subspace are clustered into regions of different thermochemical equilibrium. A classifier is then trained to classify new points into these regions. Finally, reaction kinetics and transport species are learned for each cluster by artificial neural networks.

The main tasks of the thesis are to (1) implement the proposed machine learning-based method, and (2) compare the accuracy and speed of the proposed method compared to solving the reacting flow equations, chemical kinetics and transport phenomena directly.



Temporal evolution of the thermodiffusive instability of a premixed hydrogen-air flame (blue - unburnt gas mixture, red - burnt gas mixture). Flame movement is from the right to the left.

You ...

- ... are interested in CFD (computational fluid dynamics).
- ... have previous experience in C++ (flow simulation code) and Python (machine learning).
- ... are eager to learn new skills and are able to work in an independent manner.

If you are interested, please contact:

Contact:	Borja Pedro Beltrán, M.Sc.	Mario Rüttgers, M.Sc.
Room:	004	108
Tel.:	+49 - (0)241 - 80 - 94821	+49 - (0)241 - 80 - 90396
Mail:	b.pedro@aia.rwth-aachen.de	m.ruettgers@aia.rwth-aachen.de

Lehrstuhl für Strömungslehre und Aerodynamisches Institut
Wüllnerstr. 5a, 52062 Aachen