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Master thesis – Application of artificial neural networks to predict the chemical process in combustion systems

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Problem description:

In numerical simulations of combustion processes, commonly using Computational Fluid Dynamics (CFD), a simplified approach is preferred to predict the gas phase combustion in order to save computational time. This approach only considers only a few reaction steps (e.g. a 3-step mechanism) to calculate the oxidation of methane (in Austria the main component in natural gas) to H2O and CO2:

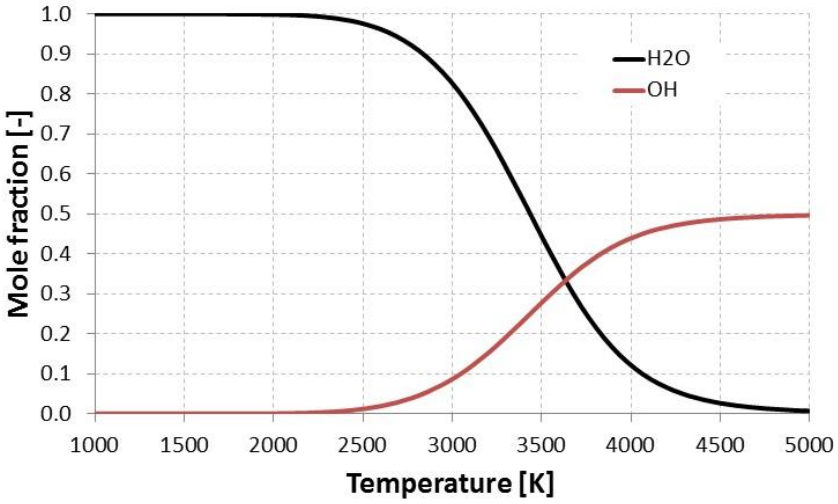
$$CH_4 + 1.5\ O_2 \rightarrow 2\ H_2O + CO$$

$$CO + 0.5\ O_2 \rightarrow CO_2$$

$$CO_2 \rightarrow CO + 0.5\ O_2$$

Considering only the reactions (called global reactions) above, important intermediate reaction (elementary reactions) steps are neglected. Such a reaction, for example, can be the dissociation (breakup) of H2O molecules in OH and H radicals due to the high temperatures in the main reaction zone of a flame. Especially when methane or hydrogen is burnt with pure oxygen for high temperature applications these intermediate reaction steps has to be taken into account. In the following chart the dissociation of H2O in OH and H radicals at high temperatures is displayed based on calculations considering thermodynamic equilibrium. It can be seen that the H2O concentration starts to decrease above 2300 K, since the H2O molecule breaks up.

$$H_2O \rightleftharpoons OH + H$$



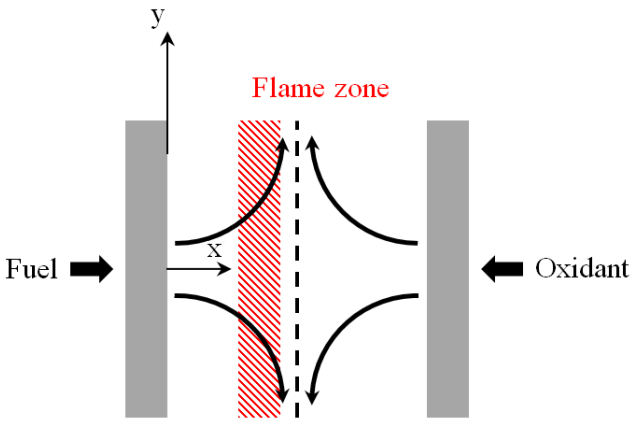
Anyway, to predict the chemical reactions during the combustion process with global reactions, it is inevitable to "adapt" the kinetic parameters of these few reaction steps. The reaction kinetic describes the transient progress of the chemical reactions in the flame. At the moment reaction mechanisms with up to 56 species (CH4, CO, CO2, H, OH, CH3, etc.) and 325 elementary reactions are in use at the Institute of Thermal Engineering (IWT). As a consequence, the computational demand is quite high for a complete simulation of a flame using CFD.

Basic question:

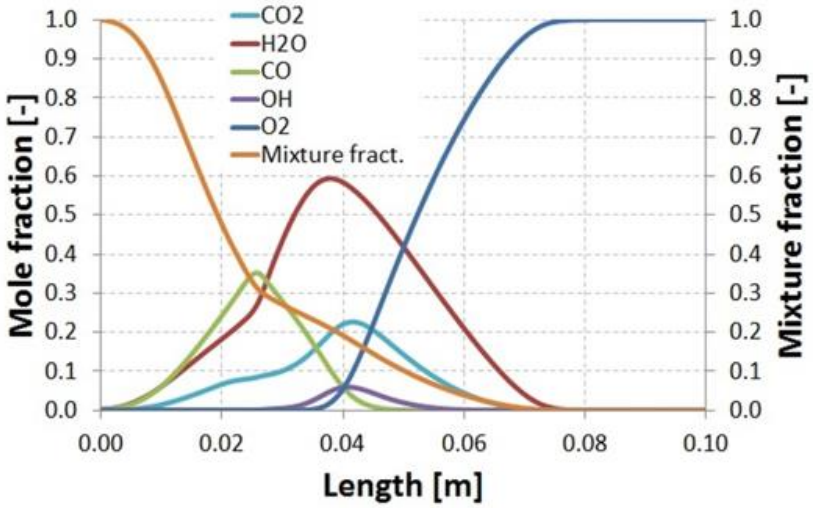
Are artificial neural networks capable to predict temperature and species concentrations in a flame, without solving an entire reaction mechanism?

Setup for the task:

To check the applicability of neural networks for the chemical reactions in the flame, the setup of a laminar counter-flow diffusion flame should be used (see following figure). Here, the fuel and oxidant (e.g. N2/O2 mixture) are transported to the reaction zone through porous media, developing an elongated flame. Such a test rig is under construction at the IWT.



The advantage of this configuration is that the chemical reaction, fluid flow etc. can be considered as 1D, and, subsequently, reaction mechanisms with more than 300 reactions can be easily investigated with a low computational demand. Therefore, case studies to generate training data for a neural network can be carried out numerically within minutes. For example, such calculations were already performed for the combustion of CH4 (from the left side) with pure oxygen O2 (from the right side) (see following figure). The distance between the fuel and oxidant inlets was 10 cm. In the figure the concentrations of several species are displayed (CO2, H2O, CO, OH, O2). The question is, can the neural networks predict the trends depending on different operating conditions?



Primary tasks:

Create neural networks to predict the calculation results of a reaction mechanism in a counter-flow diffusion flame. Prediction of the trends for the species concentrations, as given in the figure, and the temperature.

- Input data: Fuel mixture (CH4, H2, CO, etc.), oxidant mixture (N2/O2 ratio), mass-flows, radiation loss
- Output data: Trends for the species concentrations and temperature in the flame

Additional tasks:

- Find input parameterst o achieve specified output parameters. For example: Maximum temperature in the flame without exceeding a pre-defined NOx level. Which operating conditions can achieve these goals?
- Optimization of existing reaction mechanism: Identification of elemantary reactions, which have minor effects on the calculation results (sensitivity analysis).