

Uncertainty quantification of chemical kinetics for Moderate or Low-oxygen Dilution (MILD) combustion

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Introduction

Simulation of combustion processes are becoming more and more crucial in the development of new and cleaner methods for energy production. Computational Fluid Dynamics (CFD) is more cost effective compared to experiments, but the confidence in the results needs to be improved. For conventional combustion, development and validation of numerical models have been conducted for different cases throughout the last decades, but for non-conventional combustion processes (such as MILD combustion) there is still a lot of work to be done. The chemical kinetics used today for example have been optimized and validated for conventional combustion, but for non-conventional combustion regimes, the performance is still lacking. The focus of this work is therefore to improve the reliability of chemical kinetics for non-conventional combustion.

Chemical kinetics today are typically based on conventional combustion and derived from experimental data, theoretical calculations and estimations. This introduces a lot of uncertainties in the modelling, especially for non-conventional combustion where a detailed chemical mechanism is necessary to capture the slow reacting combustion zone. A detailed chemical mechanism means a lot of inherent uncertainties from the kinetic parameters, i.e. the Arrhenius constant A , the temperature exponent n and the activation energy E . The objective of this work is to reduce these uncertainties through the use of uncertainty quantification.

Methodology

The experimental and numerical work from Sabia et al. [1] was used to evaluate a Plug Flow Reactor (PFR)

during MILD conditions. To evaluate this system, the simulation software OpenSMOKE++ [2, 3] was used to analyze the effect on the ignition delay time at different conditions, which is defined as the time where the temperature is 10 K higher than the inlet temperature [1]. Based on evaluation of different chemical mechanisms in [4], the POLIMI C1-C3 (Version 1412, December 2014) [5] chemical mechanism for high and low temperatures was used for the simulations. The simulation was set up with the PlugFlow solver as a Non-Isothermal reactor with a length of 1.4 m, and an inner diameter of 0.01 m. The global heat exchange coefficient was estimated by Sabia et al. [1] to be 2.4×10^{-3} . At the inlet, methane was diluted with nitrogen, to get a 85% dilution level. The mixture was injected at a velocity of 35 m/s at a C/O ratio of 0.025. The inlet temperature of the mixture was evaluated at temperatures of; 1200, 1250, 1300, 1350 and 1400 K. To determine which parameters that had the highest uncertainty and impact on the ignition delay time, a sensitivity analysis with respect to temperature at the moment of ignition was performed. Based on this, a set of simulations were performed at $\pm 20\%$, $\pm 10\%$ and $\pm 5\%$ of the uncertain parameters. This data was then used to create a response surface with the help of the Matlab toolbox ooDACE [6, 7]. The function for the response surface was further used to find a set of values of the uncertain parameters, that gave an ignition delay time, which was within the experimental uncertainty bounds. This can be described mathematically as:

$$l_b \leq M(\mathbf{x}) - d_e \leq u_b \quad (1)$$

where $M(\mathbf{x})$ is the model response surface depending on uncertain parameters in vector \mathbf{x} , l_b and u_b are the lower and upper bounds of the experimental data d_e . This is the so called Bound-To-Bound method described in for instance [8]. The new set of parameters were then used

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during different conditions, to validate it against other measurement data.

Results and discussion

The primary sensitivity analysis, with respect to temperature at moment of ignition, indicated reaction $O_2 + CH_3 = O + CH_3O$ to have the highest sensitivity coefficient. From the chemical kinetics, the standard kinetic parameters were extracted as:

Table 1: Kinetic parameters; Arrhenius constant (A), temperature exponent (n) and activation energy (E)

Reaction number	A	n	E
229	4×10^9	0	2.7×10^4

As can be seen in Table 1 the temperature exponent (n) is zero for this reaction. The Arrhenius constant (A) and the activation energy (E) were therefore changed to evaluate the impact they have on the ignition delay time. From the response surface seen in Figure 1 below, it is clearly seen that the activation energy has a much larger impact on the ignition delay time than the Arrhenius constant.

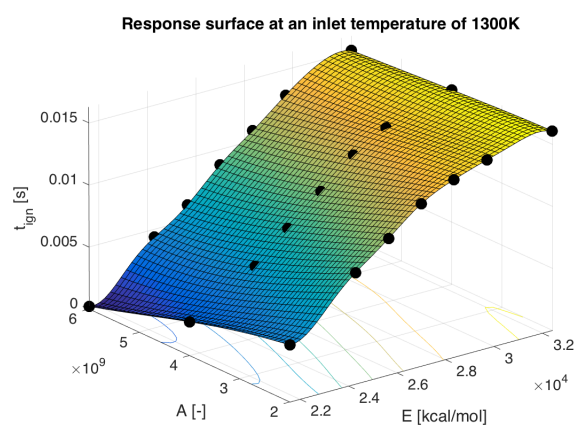


Figure 1: Response surface with respect to variations in A and E at an inlet temperature of 1300 K. The black dots represents the sampled simulation results.

With respect to the upper and lower bounds of the experimental data, the chemical kinetics was optimized considering the set of different inlet temperatures. Simulation results with the prior and the optimized mechanisms, as well as the experimental data, are plotted in Figure 2.

It can be noticed that the optimized kinetics performs better for low inlet temperatures, but for high inlet temperatures the standard kinetics are performing better.

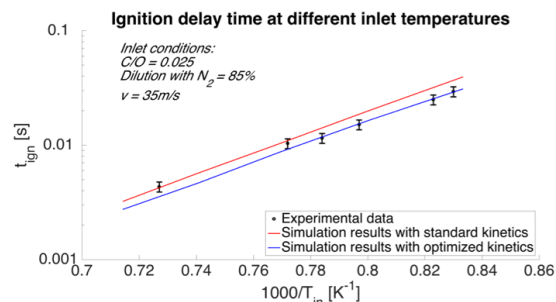


Figure 2: Ignition delay time at different inlet temperatures with standard and optimized kinetic mechanisms.

Conclusion

Optimization of uncertain parameters for non-conventional combustion regimes is crucial in order to improve the reliability of the simulation results. By utilizing uncertainty quantification, the error between the measurements and the simulation results can be minimized to a point where the simulation uncertainty is equal to that of the experimental uncertainty. The more parameters that is included in the optimization process, the better the model will perform. For further work, more experimental data, and an increased number of parameters will be included into the optimization process. This will ensure a chemical mechanism that performs better for non-conventional combustion processes.

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