Challenges in kinetic optimization

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Computational fluid dynamics (CFD) is an important tool for designing and optimizing combustion systems. However, CFD modeling of industrial combustion applications is a computationally demanding task. Today the integration of kinetics into turbulent flame simulations is one of the most difficult challenges in the combustion community. Numerous methods have been proposed for integrating kinetics into turbulent reaction flow, such as tabulation ideas [1] and trajectories in composition space [2]. However, run-time and computational power becomes a more difficult issue when such methods must be used in unsteady simulations such as hybrid URANS/LES and LES models where the conservation equations must be solved at each time step. For this reason, it is often necessary to apply simplified reaction mechanisms to reduce the computing effort. Given a detailed mechanism for a specific fuel mixture, a global mechanism can then be generated for a wide range of operating conditions matching any number of combustion parameters. To simplify the reaction mechanism it is necessary to determine which parameters may be important for the specific combustion case. For example, when generating a global mechanism for use in premixed CFD simulations, laminar flame speed is important. Other parameters may be important, such as the species production rates, the temperature and the species concentrations at equilibrium, the residence time for ignition and the 1D profiles for species and temperatures for a wide range of initial temperature, ϕ and pressures.

Zero-dimensional models, such as the Perfectly Stirred Reactor (PSR) for example could be used to describe correctly the equilibrium state which implies adequately reproduce temperatures and species concentrations at equilibrium, and to predict the residence time for ignition [3]. One-dimensional models, such as the laminar flame speed model for example, could be used to match the laminar flame speed, temperature and 1D profiles for species and temperatures [4]. In previously work by Abou-Taouk et al. [4] has an optimization strategy been used where the software CHEMKIN for chemistry is coupled with the optimization toolbox mode-FRONTIER, to end up with the best fit of the Arrhenius coefficients (activation energy, temperature exponent, reaction orders and pre-exponential factor). In practice, starting from a given set of these Arrhenius parameters, the chemical trajectories are computed using the detailed chemistry and results are stored. Then, the same points are simulated with the global reaction mechanism, the difference to the detailed chemistry solution is measured with an objective function. A new set of Arrhenius coefficients is then determined to minimize the objective function. Finally, the process is repeated and new trajectories are computed with the global reaction mechanism up to convergence.

The MILD combustion regime is based on strong EGR combined with air preheating which generates relatively low flame temperatures and thus significantly reduced reaction rates. These effects implies that the assumption of fast chemistry is not valid, [5]. The questions that arise are which parameters that are most important when it comes to MILD combustion and which models one should use in the optimization method in order to reduce the number of reactions and species. Based on the PSR model an optimization loop was performed to develop a four-step global reaction mechanism, called AAT4NR [6], with the aim to predict

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a fuel mixture consisting of 24.2% CH_4, 21.6% CO_2, 2.0% O_2 and 52.2% N_2 by volume. The validity of the mechanism is limited to atmospheric pressure, inlet temperatures from 295 - 1000 K and ϕ from 0.15 to 1. The optimized Arrhenius rates captures well the major species, the laminar flame speed, the flame temperature and the ignition delay time compared to a detailed mechanism [6]. The AAT4NR mechanism has been tested in the Delft jet-in-hot coflow (DJHC) burner [7]. Ansys CFX with RANS modeling and the combined finite rate chemistry/eddy dissipation model has been used. Figure 1 and 2 show temperature, velocity and kinetic energy profiles using different global mechanisms. The AAT4NR mechanism shows an improved prediction compared to the tested mechanisms.

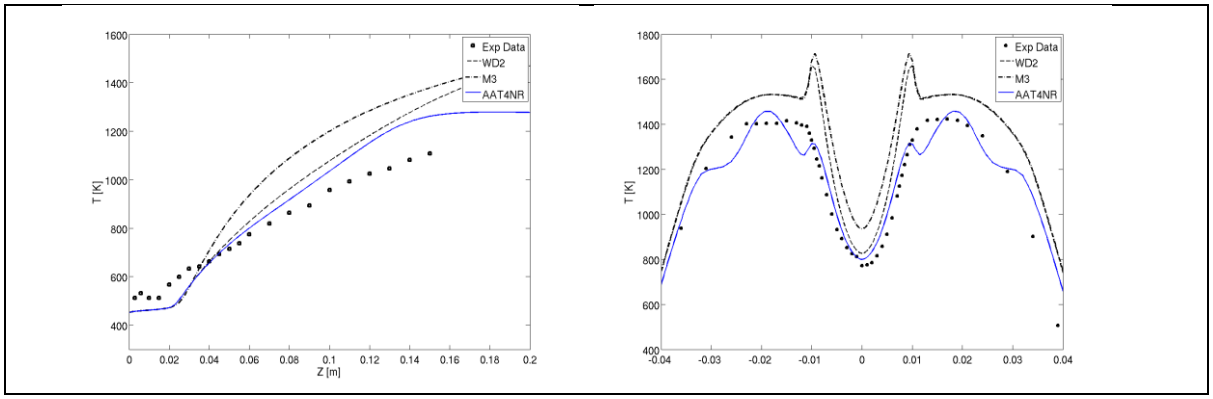

Figure 1. Temperature profiles: Left-centerline, right Z=60mm

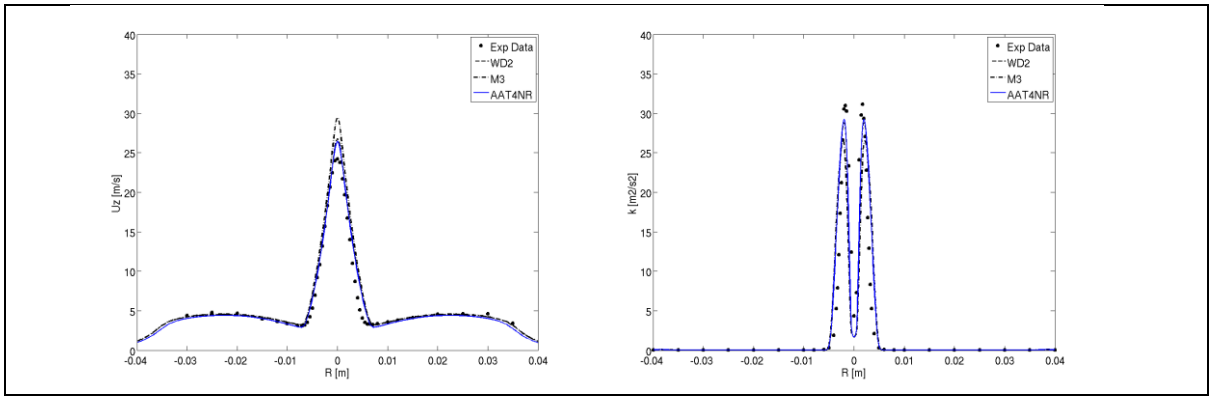

Figure 2. Left: Axial velocity at Z=30mm, right: kinetic energy at Z=15mm

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