Emerging methodologies for the co-development of simulations and experiments to reduce uncertainty in data interpretation

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Abstract

Flat flames operated at low pressures are a widely used for investigation of fuel chemistry and pollutants emerging during combustion. The presumed one-dimensionality of such flames makes them a convenient subject to detailed simulations including transport effects and reaction kinetics. However, it is observed in experiment and simulation that the probing and the geometric features of the experimental apparatus have a non-negligible impact and lead to strong deviations from one-dimensionality and the assumption of adiabatic conditions. While the deviations from the adiabatic assumption can be accessed by careful temperature measurements, the impact of the probe suction, of the buoyancy and of the apparatus geometry on the flow field remains unknown. These perturbations have a notable impact on the uncertainty in data interpretation, but can be quantified in two- and three-dimensional flow simulations [1-4].

In this work we present a comprehensive investigation of an experimental setup by means of numerical simulation of a reactive flow. In the burner chamber a home-made McKenna type flat flame burner is mounted onto a positioning system that moves the burner relative to the sampling probe. The burner can be moved up and down to change the distance between burner surface and probe and sideways to change the distance from the burner centerline to the inlet. All motion is computer controlled and accomplished using translational stages driven by stepper motors. The burner chamber has several quartz windows to allow for optical access and several additional ports for igniter, pressure gauge and thermocouple access. The burner chamber can be pumped down to 0.5 mbar using a rotary pump. Operating pressures between 10 and 1000 mbar are maintained by a computer controlled butterfly valve. The gas flow of the burner is from bottom to top so that the hot flame gases impinge on the sampling probe. Consequently, the probe has to be mounted in a cooled flange and needs to be able to withstand flame temperatures. The sampling probeis made from Hastelloy instead of the customarily used quartz of sampling probes in other flame-sampling experiments. The gases are transferred to the mass spectrometer through differently pumped chambers and analyzed by time-of-flight mass spectrometry. Mass signals are quantified by calibration measurements and result in species mole fractions. In burner scans, the burner is moved relative to the sampling location yielding concentration profiles that can be compared to simulations of the species concentrations in the laminar flame using simulation software such as Chemkin or Cantera and a detailed reaction mechanism.

The simulations of the burner chamber are performed at different levels of detail. First, three-dimensional models which consist of all aerodynamically relevant features of the setup are investigated using a strongly simplified model of the flame [1,5]. Based on these

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simulations, modifications of the burner chamber can be suggested, which would reduce avoidable signal variation due to flow field effects. The results also determine the extent of the computational domain in the second part of the investigation for simulations which include a finite rate chemistry model in 2-D and 3-D with a detailed species transport model. The temperature, velocity and species concentration fields calculated in the second step provide a quantitative measure of the experimental uncertainty, if compared to simple, one-dimensional models of the flame. However, these simulations may require the use of a skeletal, reduced reaction mechanism in order to lower the computational effort. In such a case, the computed temperature and velocity field are extracted along the axial stream line as input for 1-D simulations of the flame with a detailed reaction mechanism. The procedure is performed for different burner positions to cover the geometric variations. Finally, the simulated species concentrations are compared with the measured species profiles.

The described simulation strategy has shown to be robust and could reproduce the experimental conditions for simple fuels (hydrogen or methane) with a high accuracy [2,4]. In particular, it was found that the temperature and velocity field determined from simulations using a detailed species diffusion model and finite rate chemistry are quite insensitive to uncertainties of the reaction mechanism. Thus, we suggest such detailed simulations as a complementary tool to assess the extent of signal pertubations in experimental work relying on invasive probing techniques in the investigation of reaction mechanisms.

References

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