Compensating deviations from one-dimensionality in flame experiments by direct numerical simulation

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Experiments for the investigation of chemical reactions and their kinetics are usually designed in a way that simplifies modeling, i.e., a reduction of the set of conservation equations describing the reacting flow into a set of coupled ordinary differential equations. Typical zero- and one-dimensional experiments include shock tubes, stirred reactors, ignition bombs, rapid compression machines, or flat flames. The measurements in such devices are performed by invasive gas probing or by non-invasive laser diagnostics. Nevertheless, even for non-invasive measurements, the experiments are often performed in a confined space and the presence of surfaces has an impact on the flow and temperature field. These perturbations by invasive probing and non-ideal boundary conditions are a notable source of uncertainty in the development of reaction mechanisms and need to be quantified [1,2].

In our work we present strategies how direct numerical simulation of laminar reacting flows can be used to quantify the deviations from the assumption of an adiabatic, one-dimensional flow. In the present example, experiments are performed for a flat flame producing iron-oxide particles from iron pentacarbonyl. The 2-D and 3-D simulations are used then for quantification of the deviation from one-dimensionality in order to improve an existing reaction mechanism for iron-oxide formation [3,4]. Depending on the complexity of the reaction mechanism, a two-step simulations strategy [1] is employed by extracting temperature and velocity field from 2-D or 3-D simulations for single stream lines.

Further examples of assessment of “one-dimensional” experiments are given for a H_2/O_2 flame in a confined housing and for a sooting flame with sampling in the stagnation point [5]. The results demonstrate the value of the additional modeling effort to quantify the uncertainty introduced by deviations from ideal experimental conditions.

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