Hierarchical Models for the coupling of chemical reactions, molecular transport and flow

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Reacting flows are of great importance in many power engineering applications. A few examples are: Combustion processes, exhaust gas cleaning processes, chemical energy storage, etc. They are governed by a complex interplay of chemical reactions, flow and transport processes and can be described mathematically by solving the conservation equations for mass, momentum, energy and particle masses. These conservation equations form a large system of stiff partial differential equations and their solution represents a major challenge. Even the description of simple chemical reaction systems leads, e.g., to reaction mechanisms with over a thousand chemical species (and thus over a thousand partial differential equations), which may react in more than ten thousand elementary reactions. These kinetic processes cover time scales from nanoseconds to seconds or even hours. A similar scaling problem exists for the length scales. For example, in large technical systems, system dimensions are in the meter range, while typical reaction zones or small turbulent vortex structures are in the order of millimeters. These scaling problems are beyond the capacity of even the fastest high-performance computers when attempting to resolve the smallest scales in the numerical discretization for practical applications.

One way out of this problem is to use simplified sub-models. The mathematical modeling of reacting flows therefore raises the question of how detailed, i.e., down to which scales, the individual processes (chemical reaction, chemical-turbulence interaction, molecular transport processes) must be resolved to enable a reliable description of the overall process. The aim is to develop overall models that are as simple as possible (in terms of efficient description) but also as detailed as necessary (in terms of reliability). In particular, an oversimplification of the coupling processes between the chemical reaction and the turbulent flow, as is often the case in commercial CFD (computational fluid dynamics) applications, must be avoided under all circumstances if the mathematical modeling should possess prognostic power. We discuss how a hierarchical approach can be used to solve this problem: reduced models can be derived from detailed simulations in connection with mathematical analyzes of the dynamics of the reactive flow, which can then be used as sub-models in the description of technical systems. In this way, information about the processes on the smallest time and length scales is included in the global models. Using various examples, it is made clear that such hierarchical concepts allow a reliable description of reacting flows in mathematical modeling of processes in energy technology.