

Accelerated simulations of 1D laminar flames with detailed chemistry via operator-splitting

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One-dimensional (1D) simulations of laminar flames are a fundamental tool in combustion research, enabling the accurate computation of flame speeds and other flame properties based on detailed chemical kinetics. However, the use of fully-coupled solvers, where all governing equations are solved simultaneously, becomes increasingly impractical as the size of the kinetic mechanism and the spatial resolution grow. In such cases, the solver must manage thousands of tightly coupled nonlinear equations, leading to severe computational bottlenecks, high memory consumption, limited robustness, and reduced flexibility in parallel execution and numerical optimization [1]. This limitation is particularly critical in applications requiring the repeated evaluation of flame speeds using very large kinetic mechanisms, such as the prediction of flammability limits for sooting fuels [2].

To overcome these limitations, we adopt an operator-splitting strategy, which, though not new in the context of 1D reacting flows, has proven to be a robust and efficient approach for handling large, stiff systems arising from detailed chemistry [3]. The key innovation of our solver lies in the integration of two complementary acceleration techniques that significantly reduce computational time while preserving accuracy. The first is cell agglomeration, a dynamic procedure in which cells exhibiting similar chemical behavior are lumped together for the purpose of reaction step integration, thereby reducing the number of independent stiff systems to solve. The second is on-the-fly mechanism reduction, also known as Adaptive Chemistry Reduction (ARC), which locally simplifies the kinetic mechanism in space and time by retaining only the species and reactions necessary under current thermochemical conditions. These features provide a powerful framework for enabling fast and reliable laminar flame simulations with arbitrarily large kinetic mechanisms.

These enhancements yield a robust and flexible simulation tool, implemented within the OpenSMOKE++ framework [4], that significantly reduces computational cost and memory requirements while maintaining the fidelity of the original detailed chemistry. Benchmark tests demonstrate that the solver can handle kinetic mechanisms with thousands of species and reactions in relatively short wall-clock times, making it feasible to perform parametric flame speed studies or construct flamelet libraries even with state-of-the-art kinetic models.

References

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