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Comparisons of Chemical-Diffusive Models for Constant and Variable Stoichiometries in Navier–Stokes Simulations of Gaseous Hydrogen–Air Detonations

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The Chemical-Diffusive Model (CDM) is a reduced-parameter methodology for representing chemical reactions and energy release in numerical simulations of flames and detonations. Developing a CDM involves identifying a specific set of combustion properties for a target system (such as combustion wave velocities and temperatures) and using an optimization procedure to determine a minimal set of reaction parameters that reproduces these properties in full reactive Navier–Stokes simulations [1]. Here, we compare two versions of the CDM. The first is a standard version derived for a homogeneous, stoichiometric mixture, with fixed CDM parameters applied throughout the domain [2]. The second is an approach with spatially and temporally varying equivalence ratio (ϕ), in which ϕ is computed locally and CDM parameters are dynamically updated in each computational cell. The test problem is a detonation wave propagating in a gaseous hydrogen–air mixture. This mixture was selected for its high reactivity, practical relevance, and increasing interest for use in future propulsion and energy systems. Prior studies have shown that the standard version of the CDM can accurately reproduce detonation structure and deflagration-to-detonation transition (DDT) behavior [3, 4, 5]. In this study, we examine both versions of the CDM to determine which approach yields more accurate and computationally efficient results for large-scale detonation simulations. The aim is to compare how the two simulations differ in terms of energy release structure, flame–shock interaction, and detonation cell size, particularly in mixtures with spatially varying composition.

References

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