Effects of Isothermal Wall Boundary Conditions on DDT Simulations in $CH_4/H_2/O_2$ Mixtures in Smooth Channels

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Abstracts

Hydrogen-enriched methane mixtures are gaining attention as a transitional low-carbon fuel to support the shift toward a hydrogen-based economy, but their increased reactivity due to hydrogen addition raises critical detonation safety concerns [1]. Our recent investigation has focused on DDT phenomena in smooth narrow channels under adiabatic wall conditions using numerical simulations with the *detonationFoam* solver [2]. Results demonstrated the strong influence of hydrogen content on flame acceleration, DDT run-up distance, and detonation cell sizes. Building on the aforementioned study, the present work-in-progress examines the transition from adiabatic to isothermal wall boundary conditions for the same mixtures, aiming to better approximate scenarios encountered in practical devices. Simulations are conducted using the CKL 1.1 detailed chemical mechanism for three stoichiometric $CH_4/H_2/O_2$ fuel blends with varying hydrogen content (50%, 66%, and 80%). Previous adiabatic-wall simulations demonstrated that all three $CH_4/H_2/O_2$ mixtures undergo DDT via a few distinct mechanisms—such as ultra-fast flame formation, tongue-shaped flame collapse, or hotspot-triggered ignition. In contrast, introducing wall heat loss via isothermal boundaries fundamentally could alter the thermal condition and flame structure of the near-wall region, where energy loss suppresses local reaction rates and impedes the formation of flame structures critical to DDT initiation [3]. This study investigates whether DDT in hydrogen-enriched methane mixtures can still emerge under isothermal wall boundary conditions and how the flame–shock dynamics deviate from the adiabatic baseline, contributing to a refined understanding of wall-thermal effects in reactive flows and on DDT.

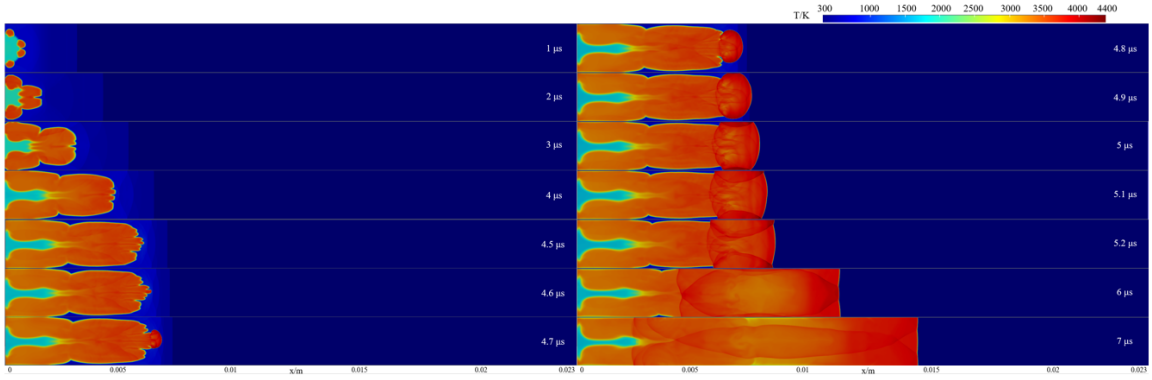

Figure: DDT in a stoichiometric H_2/O_2 mixture in a channel with isothermal cold wall $T = 300$ K

References

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