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Numerical investigation of Hydrogen self-ignition and deflagration-to-detonation phenomena using automated meshing approach and detailed chemistry

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Computational fluid dynamics (CFD) plays a critical role in designing safe storage and transport systems for hydrogen. Fine mesh resolution and detailed chemistry are essential to the accurate prediction of self-ignition and deflagration-to-detonation (DDT) in hydrogen air mixtures. However, simulating H2 venting and explosion in real life scenarios (complex obstacle shapes and large computational domain) involves tedious meshing effort and several mesh iterations to refine flame and shock locations. Towards addressing these challenges, the capability of a detailed chemistry approach combined with automated meshing based on cut-cell technique and adaptive mesh refinement (AMR) is assessed.
Furthermore, three different turbulence-chemistry interaction modelling approaches are critically compared – a homogeneous reactor model, an eddy dissipation concept and a three-point PDF approach.

Two configurations are studied: First, the phenomena of self-ignition of hydrogen as it exits from high pressure vessels [1]. A set of experiments are modeled numerically to evaluate the condition in which the hydrogen stored in high pressure vessels can self-ignite as it exits a narrow tube. The effect of obstacles is investigated for various tube diameters and tank pressures. Second, the DDT in hydrogen rich enclosures is evaluated [2, 3]. The numerical investigation is configured to replicate the experimental investigations on DDT of hydrogen within enclosures. The effects of homogenous and inhomogeneous gas distribution conditions and buoyancy effects are considered.

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