Preferential diffusion effects on tabulated chemistry methods for hydrogen/methane and hydrogen/ammonia blends

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Abstract
Advancements in more efficient combustion systems heavily rely on understanding the fundamental combustion characteristics of the different energy carriers and numerical simulation has a fundamental role in that. However, detailed chemistry simulation can be computationally prohibitive for industrial design workflows. Tabulated chemistry methods stand out as a promising approach, offering a cost-effective method for maintaining accuracy in simulations. Manifold generation is a pivotal aspect of tabulated chemistry methods as it delineates the range of thermochemical states accessible during the simulation. Preferential diffusion is one of the dominant effects that must be included when hydrogen is used as a fuel. The present work aims at numerically investigate the effect of preferential diffusion on flamelet-generated manifolds for different hydrogen-methane and hydrogen-ammonia blends. Extinguish counterflow diffusion flames are used for the generation of the manifold, solved by CHEM1D with two different transport models. As expected, preferential diffusion effects are predominant at high hydrogen molar fractions and become negligible at concentrations lower than 0.5. Preferential diffusion affects the shape of the manifold, i.e. higher diffusion of the progress variable species towards leaner and richer mixture fractions. Contours of the progress variable source term show higher peaks for the unity-Lewis case, due to the absence of diffusive transport, while a wider reaction zone is observed for the mixture-averaged case. Hence, manifolds are deeply affected by preferential diffusion, emphasizing the necessity of its incorporation into flamelet equations.

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