A simplified thermodynamically-consistent single-step mechanism for hydrogen combustion

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In recent years, significant efforts have been dedicated to developing a reduced single-step formalism for hydrogen combustion [1–3]. While reduced mechanisms mitigate stiffness and computational cost [4]. many still fail to accurately capture adiabatic flame temperature T_{ad} (overestimation by 200 K) near stoichiometric conditions in H_2/air flames. Millán-Merino and Boivin [1] demonstrated that a single-step mechanism with a variable stoichiometric coefficients formalism is able to recover T_{ad} by embedding thermodynamic equilibrium constraints directly into these coefficients. We propose a simplified formulation of this mechanism (1) by only retaining the contribution of the OH radical among dissociation products, neglecting the contributions from radicals H and O initially considered in [1] :

$$\nu'_{\mathrm{H}}\mathrm{H}_2 + \nu'_{\mathrm{O}}\mathrm{O}_2 \xrightarrow{\omega} \nu'_{\mathrm{H_2O}}\mathrm{H_2O} + \nu'_{\mathrm{OH}}\mathrm{OH} \tag{1}$$

The global reaction rate ω is of the form $\omega = \lambda\zeta$, where λ is a characteristic inverse branching time associated with the chemistry of premixed flame. ζ is a concentration accounting for H, O and OH species growth. In this study, all results are obtained using mixture-averaged transport.
Results show that the model has equivalent accuracy (both in terms of flame speed S_L and T_{ad}) than the full 7-species model [1] for a wide range of equivalence ratio (0.4-10) and pressures (0.5-20 atm). A clarification of the role of variable stoichiometric coefficients is also provided, including the analytical derivation of a first-order approximation that improves stability and convergence in flame simulations. Going forward, further validation will focus on quantifying the robustness of the approach in multi-dimensional CFD simulations. Future work will also investigate a potential extension of this methodology to non-diluted hydrogen combustion.

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References

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