



Including pollutant prediction within a standardized virtual chemistry framework

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The combustion modeling of decarbonized fuels, such as sustainable aviation fuels, presents significant scientific challenges due to their intricate chemistry. Detailed kinetic mechanisms, involving thousands of species and reactions, lead to prohibitive computational costs for multidimensional turbulent simulations of combustion chambers. To address this issue, various chemistry reduction techniques have been developed, with virtual chemistry emerging as a particularly efficient method. This approach consists in building highly-reduced chemical schemes, using virtual species and reactions with optimized thermochemical and kinetic properties to accurately reproduce selected flame characteristics [1]. Although particularly performant in modeling pollutants such as NO_x [2] and soot [3], the original formalism of virtual chemistry includes special features that deviate from classical chemistry requiring source code modifications in traditional reactive flow solvers.

The present work relies on a novel virtual chemistry framework that leverages total and equilibrium reactions to link real and virtual species. Optimized to reproduce the thermal flame structure and flame consumption speed across various operating conditions, the resulting highly-reduced virtual schemes systematically recover detailed chemistry macroscopic flame properties while keeping their standard CANTERA/CHEMKIN thermodynamic and kinetic structures. Building on this foundation, an additional optimization step is here introduced to model the production of any desired pollutant through the recovery of its source terms and equilibrium mass fractions. Applied to original H_2 and $nC_{12}H_{26}$ virtual schemes using CANTERA's chemical equilibrium and flamelet computations, this study demonstrates the framework's potential to accurately predict pollutants such as NO. Further discussions will explore the broader applicability and generalization potential of this innovative approach, emphasizing its effectiveness for various fuels and pollutants.

References

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