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Modeling and Optimization of Virtual Chemical Mechanisms for Complex Fuels Using Cantera

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Since the development of the detailed methane (CH4) combustion mechanism GRI-Mech3.0 (GRI3.0), the tendency to expand the number of species and reactions in newer hydrocarbon mechanisms has introduced a computational bottleneck for CFD reactive flow analysis. The sheer amount of data to be processed, stored, and exchanged per cell and per timestep by the solver (or coupled solvers) makes some fuels too demanding for current industrial simulations, especially when simulations involve millions of cells in high Reynolds condition. This has motivated academic works aiming to simplify such models by reducing their size (e.g., via DRGEP or SA techniques) or by bypassing the complexity using tabulation methods like ISAT.

A novel method introduced by Cailler in 2018, called Virtual Optimized Chemistry [1], proposes a simplification strategy. By tuning molecular weights and adjusting both thermodynamic and kinetic properties of the fuel, oxidizer, and diluent under simplified assumptions, a virtual scheme is constructed. Intermediate species are grouped into simplified reactions with properties optimized to reproduce key outputs—like temperature, flame speed, heat release rate, and pollutant formation. The method is exemplified using CH4 as a reference fuel mixture.

The current virtual chemistry model is built entirely using open-source tools and packages [2], differing from other implementations that depend on proprietary or in-house software. This approach introduces a new tool for generating such mechanisms to be coupled to CFD tools. Furthermore, more robust optimization strategies are under investigation, helping further reduce the computational cost per mechanism—even when not limited to purely hydrocarbon fuels.

Successful virtual methane mechanisms were created with this method. Through an additional optimization routine, it is now possible to create the necessary submechanisms for carbon monoxide (CO) formation, paving the way for future reactive CFD analyses with the computational efficiency of a global step mechanism, which maintains the pollutant formation accuracy of GRI3.0 for a selected range of thermophysical and mixture properties in the combustion.

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References

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