Numerical modeling of soot formation in laminar methane/oxygen inverse diffusion flames with fuel dilution

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The formation and evolution of soot nanoparticles in laminar inverse diffusion flames (IDFs) is a critical phenomenon in combustion processes relevant to hydrogen production via autothermal reforming (ATR). In this work, we perform detailed numerical simulations of recent experiments by Serrano-Bayona et al. [1], which systematically investigated the effect of various diluents (CO_2, N_2, Ar, He) on soot formation in methane/oxygen IDFs at atmospheric pressure. The numerical framework adopts a detailed kinetic mechanism from the CRECK Modeling Lab, coupled with a Discrete Sectional Model for soot, enabling accurate prediction of the formation, growth, and oxidation of soot nanoparticles and aggregates [2].

All flame configurations described in [1] were simulated with satisfactory agreement between computed and experimental trends for flame height, temperature, PAH distribution, and soot volume fraction. We perform an in-depth kinetic analysis to elucidate the role of each diluent in modifying the reaction pathways leading to soot precursors. The simulations confirm that CO_2 strongly suppresses soot formation through both thermal effects (e.g., heat capacity and flame temperature reduction) and chemical effects. In contrast, He modifies the flame structure due to its high thermal and mass diffusivity and low molecular weight, which influence temperature profiles, flame height, and the distribution of reactive species.

From a computational standpoint, the stiffness and complexity of the detailed chemistry (hundreds of species and thousands of reactions) required special attention. To reduce CPU time without sacrificing accuracy, we implemented a dynamic load-balancing strategy tailored for multidimensional simulations with detailed kinetics [3]. The approach was further enhanced by cell agglomeration, allowing us to reduce the computational overhead.

This study highlights the potential of detailed multidimensional simulations in capturing the nuanced behavior of soot formation in IDFs and demonstrates how advanced numerical strategies can mitigate the heavy computational cost associated with such models.

References

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