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An OpenFOAM-Based CFD Solver for Soot Formation in Laminar Reacting Flows

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A comprehensive CFD tool based on the OpenFOAM platform has been developed to simulate soot formation in laminar reactive flows. This tool integrates the Cantera chemistry solver via the DeepFlame OpenFOAM–Cantera coupling [1]. To model soot dynamics, the solver incorporates both Monodisperse and Sectional Population Balance Models (MPBM and SPBM). The MPBM, implemented within a CFD framework for the first time, offers a computationally efficient alternative for tracking soot evolution. When particle inception and surface growth are rapid, and high particle concentrations lead to the emergence of self-preserving size distributions, the MPBM provides accurate predictions of average particle properties. In contrast, the SPBM–while more computationally intensive–resolves the particle size distribution and captures the evolution of soot morphology and composition with high fidelity. Both models track key variables such as agglomerate and primary particle number density, total carbon, and hydrogen content, enabling detailed predictions of soot yield, structure, and composition.

The framework also includes a wide selection of inception and surface growth models from the literature, offering flexibility to test different theoretical formulations and physical mechanisms. To enable high-fidelity simulations of soot formation in laminar flows, the solver incorporates several essential physical sub-models, such as radiation models, conjugate heat transfer, and necessary boundary conditions. These capabilities substantially enhance the solver's applicability across various combustion scenarios. The modular architecture of the solver facilitates systematic investigation into the effects of soot inception and surface growth models.

This CFD tool has been applied to simulate a variety of benchmark laminar flames, including premixed, counterflow diffusion, and both normal and inverse coflow diffusion configurations. The simulation results have been validated against experimental data, demonstrating the predictive reliability of the model. The results highlight the importance of including buoyancy effects and accounting for radiation from both soot and gas-phase species in accurately predicting particle temperature-time histories. Furthermore, the findings indicate that not all chemical mechanisms yield accurate predictions, with the Caltech mechanism showing superior performance in capturing both solid and gas-phase properties.

References (if needed)

[1] Mao R et al. DeepFlame: A deep learning empowered open-source platform for reacting flow simulations. *Computer Physics Communications*. 2023;291:108842.