Multiphase CFD Simulation of Methane Decomposition in a Molten Bubble Column Reactor: Hydrodynamics and Reaction Coupling

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This study presents a novel 3D CFD framework for simulating reacting methane flow in a molten metal bubble column reactor, targeting high-efficiency hydrogen production through thermal methane pyrolysis. While previous efforts, such as Ngo et al. [1] addressed the hydrodynamics of molten-metal bubble columns using Volume of Fluid (VOF) methods, this work advances the field by developing a reactive Eulerian–Eulerian multiphase model that captures the interplay between hydrodynamics and gas-phase chemistry.

The model incorporates surface-catalyzed methane decomposition at the gas–liquid bubble interface along with volumetric gas-phase reaction kinetics, providing a more realistic depiction of the reactor environment. It is constructed using a RANS-based turbulence model (standard k-ε) augmented with bubble-induced turbulence dispersion and higher-order spatial discretization to enhance prediction accuracy. Bubble formation, gas holdup, species transport, and interfacial heat and mass transfer are resolved under operating conditions of 1075°C, 20 bar, and 1.16 g/s methane flow.

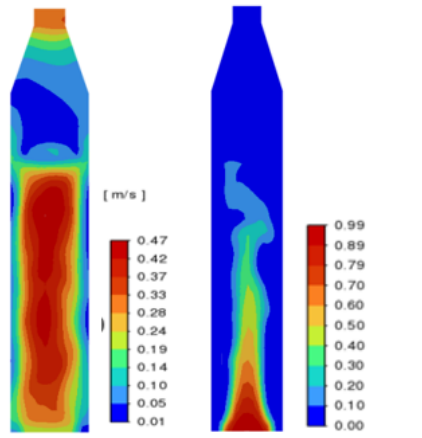

Figure: Gas velocity and CH_4 mass fraction contour profiles

Simulation results demonstrate 97.5% methane conversion, bubble diameters in the range of 5.5–7.8 mm, and bulk gas holdup ranging 0.15 - 0.3. The model was validated using benchmark experimental data from gallium-based molten methane pyrolysis systems, demonstrating close agreement with measured methane conversions reaching 81% at 900°C.

The key novelty lies in the first of its kind 3D integration of reacting gas flow, bubble-scale catalysis, and multiphase transport within a molten metal column, enabling predictive optimization of methane conversion and hydrogen yield. The modeling framework sets the foundation for design, scale-up, and performance evaluation of future pyrolysis reactors, particularly in systems where solid carbon handling, wall heat transfer, and flow stability are critical.

References

[1] Ngo, S.I., Lim, Y.I., Kwon, H.M. and Lee, U.D., 2023. Hydrodynamics of molten-metal bubble columns in the near-bubbling field using volume of fluid computational fluid dynamics. *Chemical Engineering Journal*, *454*, p.140073.