Volume-Of-Fluid Simulations of Droplet Combustion

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Abstract
This work presents a comprehensive multiphase CFD framework which allows simulations of droplet evaporation and combustion problems, without assuming spherical symmetry. The model resolves the full multidimensional set of transport equations on mass, momentum, chemical species, and the temperature of the system. The gas-liquid interface is transported using the Volume-Of-Fluid approach, while the chemical reactions and gas-phase radiation are included using a direct-integration technique. The model's validation confirms its accuracy in predicting the burning rates of droplets in microgravity conditions. More complex test cases, including the effect of normal gravity, are used to quantify the error of the spherical symmetry, especially at high Grashof numbers. Lastly, the multicomponent phase change model is exploited to resolve the droplet extinction due to water absorption effects.

Introduction
The analysis of droplet combustion is fundamental for understanding and optimizing spray combustion in burners and engineering devices. Traditional models usually assume spherical symmetry, limiting the fluid dynamics phenomena in favor of a computationally efficient model which can accommodate complex kinetics. However, these models cannot capture multidimensional phenomena like buoyancy-driven flows, droplet deformation, liquid recirculation effects, turbulent conditions, and interactions among multiple droplets. This work aims to overcome such limitations by coupling multiphase CFD models, for a detailed description of the fluid dynamics, with direct integration of chemical kinetics. This work advances the state-of-the-art by combining cutting-edge discretization techniques for phase change with the direct integration of the chemical kinetics. The resulting formulation is general and it can accommodate arbitrarily complex kinetics, compatibly with the desired computational time.

Numerical Model
The numerical model solves the low-Mach form of the Navier-Stokes equations for multicomponent systems [1,2]. These equations are approximated using a time-staggered projection method, introducing additional source terms which accounts for the gas-liquid interface boundary conditions [1,2]. The interface is represented using a discontinuous scalar marker function, representing the volume fraction of liquid in each computational cell of the domain. Using the Volume-Of-Fluid approach, the interface is transported by solving an advection equation on the volume fraction

field. The model is implemented in the open-source software Basilisk [3], which is coupled with the OpenSMOKE++ library [4] which reads the kinetic schemes in CHEMKIN format, calculates the thermodynamic and transport properties, and integrates the chemical reactions. The kinetics model used in this work is the two-step scheme proposed by Westbrook and Dryer [5], to limit the computational cost of the simulations focusing on the validation of the methodology.

Results

Simulations were conducted to validate the model against experimental data in different operating conditions, and to measure the discrepancy between the full multidimensional model and the assumption of spherical symmetry.

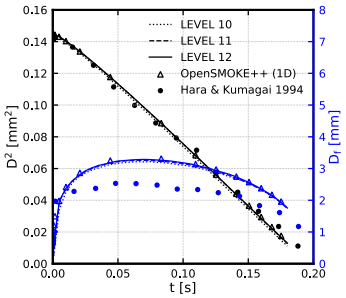

Figure 1: burning rates and flame diameter of n-heptane droplet combustion in microgravity.

The simulation of n-heptane droplets in microgravity conditions is considered to study the grid independence of the simulations, and to identify a grid refinement which can be a good compromise between accuracy and computational costs. Figure 1 shows that the burning rate from this model converges toward the benchmark 1D model from the OpenSMOKE++ suite [4], and these models also correctly capture the experimental burning rate by Hara and Kumagai [6]. Small discrepancies in the flame diameter can be attributed to differences in their definitions and the use of simplified chemical kinetics.

Ethanol droplets in microgravity conditions were simulated and compared with experimental data, capturing the burning rates accurately (not shown) and explaining the role of radiation with increasing initial amount of CO_2 in the environment.

Methanol droplets in normal gravity conditions were simulated to measure the impact of buoyancy-driven flows on the droplet consumption dynamics. Figure 2 shows a 6% deviation between the burning rates in microgravity and in normal gravity conditions for the atmospheric pressure case. As pressure increases, the deviation also grows, resulting in inaccurate predictions by spherically symmetric models (Microgravity) due to the non-negligible influence of buoyancy-driven flows. The flame upward stretching increases with pressure, and it leads to a flame front which is closer to the droplet surface. Introducing the water absorption during methanol combustion we predicted the correct qualitative behavior of droplet extinction.

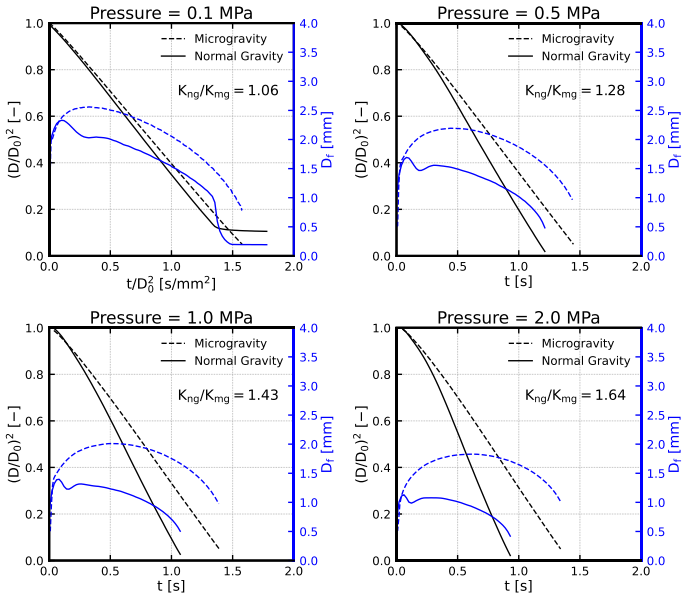

Figure 2:burning rates and flame diameters for methanol droplet combustion in normal gravity conditions, at different pressure values.

Conclusions

The model successfully couples a VOF-based phase change model with the direct integration of the combustion chemistry, accurately predicting droplet burning rates in different gravity conditions. It highlights the need for multidimensional modelling under normal gravity especially at high pressures. Future work will address fiber heat conduction, Marangoni effects, and the optimization of the computational cost.

References

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