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## Modeling of Two-phase systems: Atomization to Reacting sprays

### Abstract:

Combustion has been and currently is the major source of energy production. In the past, fossil fuels formed a primary energy source produced through combustion. The fossil fuels require millions of years to renew themselves, which would not be possible with the current consumption rate and deforestation. Additionally, they form the major source of air pollution, being a cause of respiratory problems and ecological destruction. But with the advent of new methods to harness renewable resources, there is a constant effort to shift away from fossil fuels. There remain many challenges in the path and issues to be resolved for this major shift. Though the transition to renewable resources will be gradual, a complete shift to renewable resources would not phase out the combustion from being a strong contender in energy production and usage. The fuels like hydrogen, biodiesel, ethanol-diesel blends, methanol, etc., form an important future of renewable energy sources, achievable only through a combustion process. Hence, constant research into a clean combustion process and the methods to harness energy through combustion are going to remain, especially where high-density based sources of energy are required at relatively less cost and eco-friendly manner. Technological advancement in the research of combustion processes includes many aspects, including the development of new frameworks or equipment, or methodologies to use and test the combustion processes. The work carried out in this study is one such effort.

Liquid fuel combustion involves multiple physical processes that must be modeled for a computational simulation. First, the involvement of the liquid phase along with the gaseous oxidizer (usually air) makes it a multi-phase flow that includes phenomena like atomization. Then, a phase-change phenomenon is a must for liquid fuel to convert into a gas phase and mix with the gaseous oxidizer before, finally, the combustion happens under favorable conditions. Hence, the development process involves delving into each part involving modeling or implementation. The current work attempts to develop a framework to model the aforementioned physical processes concerning a few aspects, like mesh size, higher computational efficiency, and other existing challenges.

Firstly, a large number of computational studies of the automotive combustion chambers are based on the Lagrangian simulations, Still, they tend to avoid the critical primary breakup and focus on secondary atomization. When the fuel is injected through a nozzle at high pressure into the low-pressure cylinders or is already superheated during the passage through fuel pipes before injection, it tends to undergo liquid flashing-based primary breakup. Hence, the first part of the study involves the development of a primary breakup model for a Lagrangian-based computational framework in the flashing conditions. The new model is validated against the experimental results for different fuels at different chamber pressures and superheated temperatures.

Another solution to the challenge may lie in a methodology where the dense region of a liquid jet breakup is solved in the Eulerian framework while the downstream secondary atomization is solved using the Lagrangian system, empowering the computational methodologies to simulate the industrial-scale problems. This type of methodology does not need Lagrangian-based primary breakup models for the near-nozzle region and is resolved by the Eulerian approach, thus, saving from the errors due to the modeling and its assumptions. Hence, the second part of the work focuses on developing a lone, consolidated compressible solver with the flexibility to account for every process. The new solver is validated for liquid jet-in-crossflow against the experimental database. Further analysis is carried out for three LJICF cases falling under three extreme breakup regimes by varying Weber number and momentum flux ratio. The breakup instability is observed to change from Kelvin-Helmholtz to

Rayleigh-Taylor type by varying momentum flux ratio. Similarly, behind-the-liquid-jet flowfields and bifurcations are also studied.

Finally, the combustion Flamelet Generated Manifold (FGM) model is implemented to simulate the final stage and is validated for auto-igniting methanol burner. Considering the large resources and complexities involved with the dense sprays, the dilute spray flames are chosen as an initial step for validations. Further, the analysis of the ignition kernel and flame propagation around the vortical structures is carried out using the proper orthogonal decomposition (POD) technique.