Numerical modelling of Spray Evaporation

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Polydispersed turbulent evaporating and reacting two-phase flows are challenging problems occurring frequently in industrial processes, for example spray coating and oil fired furnaces. The accurate Modelling of these types of flows and efficient numerical methods are both extremely important in order to be attractive for use in industrial practice. However, probably because of the complexity of the problem, experiments and validated simulations in this area are scarce.

A stochastic Lagrangian-Lagrangian particle (or Monte Carlo) approach is used to simulate an evaporating spray. In this approach, Stochastic differential equations (SDE's, or Langevin equations) of motion are solved for both gas particles and liquid particles. Each gas particle represents a possible state of the gas phase (velocity, composition, temperature). Each liquid particle represents a possible state of a liquid droplet (velocity, diameter, velocity seen, etc.). The ensemble of particles represents the joint velocity-composition Mass Density Function (MDF, a density weighted PDF) $\mathcal{F}_{U\phi}(x, V, \psi; t)$ for liquid and gas, see also Naud³.

A so-called hybrid method is used where a number of Eulerian transport equations are solved to close the Langevin equations, in particular terms involving pressure gradient, Reynolds stresses, dissipation and velocity seen⁴. The Eulerian equations depend on the mean density obtained from the particle method. The hybrid closure method also reduces statistical errors (bias). There is also the possibility of using a chemistry model in case chemical reactions occur. A schematic of the model can be found in Figure 1.



Figure 1: Finite Volume - Monte Carlo modelling approach

The dispersed phase is described by standard single droplet evaporation models including the infinite conductivity model, the conduction limit model and the effective conductivity model. The droplet motion is described with a transport equation for the mass density function $\mathcal{F}_p(x, V_p, \psi_p, V_s, \psi_s; t)$ instead of the usual droplet density function (DDF). This allows us to get a correspondence between local (Eulerian) and dispersed (Lagrangian) descriptions. The transport equation for the MDF is not solved directly. Instead, equivalent Lagrangian equations of motion are solved for computational particles that represent a stochastic sample of the flow¹. The above approach is used to simulate a swirling and evaporating polydispersed spray. Experimental results for a isopropyl-alcohol spray were obtained by Sommerfeld and Qiu⁵. The experimental configuration can be seen in Figure 2. Mean droplet properties (velocity, velocity fluctuation, droplet size, temperature and mass flux) were measured at six locations downstream of the inlet. At the inlet, detailed measurements were taken for several droplet size classes. A weak first order stochastic integration method is used to integrate the set of SDE's². A simplified Langevin model is used to model the dispersion, mixing is modeled by



Figure 2: experimental and computational domain for the vaporising spray

the modified Curl model and two-way coupling effects are neglected in these simulations.

Simulations were performed for several droplet vaporisation models and compared with the experimental data. The experimental data and numerical results for the infinite conductivity model can be seen in Figure 3. The figure shows radial profiles of droplet mass flux and droplet diameter at several axial locations downstream of the inlet. The numerical results show a good agreement with the experimental data along the centreline, which is due probably to more detailed measurements near the centreline. We will present a detailed comparison of experimental data and model predictions for the different droplet models.



Figure 3: experimental and simulated results for the vaporising spray.

References

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