Abstract

Numerical modeling of several turbulent nonreacting and reacting spray jets is carried out using a fully stochastic separated flow (FSSF) approach. As is widely used, the carrier-phase is considered in an Eulerian framework, while the dispersed phase is tracked in a Lagrangian framework following the stochastic separated flow (SSF) model. Various interactions between the two phases are taken into account by means of two-way coupling. Spray evaporation is described using a thermal model with an infinite conductivity in the liquid phase. The gas-phase turbulence terms are closed using the k-ε model. In the classical SSF (CSSF) approach the effects of turbulent velocity fluctuations of the gas-phase are modeled stochastically to obtain instantaneous gas-phase velocity, which subsequently is used to estimate droplet dispersion and interphase transport rates. However, in the CSSF model, no such effort is made to model the effects of the fluctuations in the gas-phase reactive scalars, namely temperature and species mass fractions. Instead, the mean value of these scalars is used while solving for the droplet governing equations and estimating various interphase source terms. Also, in flamelet model and conditional moment closure (CMC) applications of turbulent sprays, the mixture fraction is defined using conventional definition, which is no longer a conserved quantity due to associated phase change.

Therefore, in this thesis a novel mixture fraction based FSSF approach is used to stochastically model the fluctuating temperature and composition of the gas phase. These gas-phase reactive scalars are then used to refine the estimates of the heat and mass transfer rates between the droplets and the surrounding gas-phase. It is assumed that the fluctuations in the gas-phase reactive scalars are inherently associated with the fluctuation of a single conserved scalar, namely instantaneous mixture fraction. Instantaneous value of the gas-phase reactive scalars *seen* by individual droplets is then estimated from the instantaneous gas-phase mixture fraction, which is obtained as the Weiner process by randomly sampling a known beta-function probability density function (PDF) of the local mixture fraction field. Finally, Favre mean value of the gas-phase scalars are recovered as appropriate moments of the PDF. The present definition of the mixture fraction based on its instantaneous value facil-

itate exact calculation of the source terms in the transport equation for variance of the mixture fraction, whereas conventional definition leads to terms which require further modeling and simplifications. The present FSSF model also accounts for the possibility of existence of an envelope flame between the droplet and the bulk gas-phase, which greatly increases the heat and mass transfer rates to the droplet. The present model allows us to treat the occurrence of envelope flame separately which is otherwise neglected in the conventional spray combustion models.

The FSSF model is implemented into a numerical code, and different well-defined nonreacting and reacting turbulent spray jets are investigated. For the reacting spray jets, single-step irreversible reaction with infinitely fast chemistry is assumed in the body of the flow. In such cases special care must be taken with modeling the upstream boundary condition. This is because the flow from the spray jet nozzle is unreacted and yet it becomes well reacted shortly downstream. Numerical results are compared against experimental measurements as well as with predictions using the CSSF approach. Numerical results from the FSSF and CSSF model are almost identical for the nonreacting spray jets, where the fluctuations in the gas-phase scalars are relatively low. For the reacting sprays, significant differences are found between the results of the FSSF and CSSF models for the reacting spray jets, where the fluctuations in the reactive scalars are high. The FSSF model reasonably predicts many features of the jet spray flames, such as flame length, gas-phase temperature, and spray droplet velocity/diameter distribution; results appear to be close to the experimental measurements.

Finally, the combustion characteristics of the reacting spray jets are studied following classical group combustion theory. It shows that these spray jets have external group combustion mode near the nozzle-exit. Transition to internal group combustion takes place at different downstream locations based on the droplet loading and equivalence ratio at the nozzle-exit, whereas single droplet combustion regime is observed near the tip of the visible flame. Another alternate approach to study the combustion behavior of a cloud is proposed based on fraction of droplets having i) no envelope flame, ii) envelope flame, iii) extinguished envelope flame due to high slip velocity, iv) extinguished envelope flame due to droplet diameter being too small, v) both iii) and iv) above. Based on these, different group combustion behavior of the reacting spray jets are interpreted.