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Mixing and evaporation of multiple size group JP-7 fuel droplets injected into a supersonic air stream – efficiency of cylindrical versus rectangular combustion chamber

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ABSTRACT

This report deals with the formulation, implementation, and testing of three numerical techniques based on (i) a full multiphase approach, (ii) a MUlti-Size Group (MUSIG) approach, and (iii) a Heterogeneous MUSIG (H-MUSIG) approach for the prediction of mixing and evaporation of liquid droplets injected into a stream of air flowing inside a combustion chamber. The numerical procedures are formulated following a Eulerian approach, within a pressure-based fully conservative Finite Volume method equally applicable in the subsonic, transonic, and supersonic regimes, for the discrete and continuous phases. The k - ϵ two-equation turbulence model is used to account for the droplet and gas turbulence with modifications to account for compressibility at high speeds. For the purpose of comparing the performance of the various methods, three configurations involving stream-wise and cross-stream spraying in rectangular and cylindrical domains are investigated and solutions for evaporation and mixing in the subsonic and supersonic regimes for droplets sprayed in turbulent flow streams are generated. Results, displayed in the form of droplet velocity vectors, contour plots, and axial profiles indicate that solutions obtained by the various techniques exhibit similar behavior. Differences in values are relatively small with the largest being associated with droplet volume fractions and vapor mass fraction in the gas phase. This is attributed to the fact that with MUSIG and H-MUSIG no droplet diameter equation is solved and the diameter of the various droplet phases are held constant, as opposed to the full multiphase approach.

Nomenclature

$A_p^{(k)}, \dots$	coefficients in the discretized equation for $\phi^{(k)}$.
$B_p^{(k)}$	source term in the discretized equation for $\phi^{(k)}$.
B_{ij}	breakup rate.
B'_{ij}	breakup frequency.
$C_p^{(k)}$	coefficient equals to $1/R^{(k)}T^{(k)}$.
C_D	drag coefficient.
c_p	specific heat at constant pressure.
C_{ij}	coalescence rate.
d	droplet diameter.
d_s	Sauter diameter.
$\mathbf{D}_p^{(k)}[\phi^{(k)}]$	the Matrix $\mathbf{D}$ operator.
f	population fraction.
$\mathbf{F}^B$	Body force.
$\mathbf{F}^D$	drag force.
h	static enthalpy.
$h_{correction}$	correction coefficient for heat transport in droplet model.
$H_p[\phi^{(k)}]$	the H operator.
$\mathbf{H}_p[\mathbf{u}^{(k)}]$	the vector form of the H operator.
$m_{correction}$	correction coefficient for mass transport in droplet model.
$\dot{m}_d$	mass rate of droplet evaporation.
$\dot{M}_d$	volumetric mass rate of droplet evaporation.

n	number density distribution function.
P_k	production term in k and ε equations.
p	pressure.
Pr	laminar Prandtl number of fluid/phase k .
Pr_t	turbulent Prandtl number of fluid/phase k .
$\dot{q}$	heat flux.
$Q_{(k)}$	general source term of fluid/phase k .
$R_{(k)}$	gas constant for fluid/phase k .
Re_d	Reynolds number based on the droplet diameter.
S	source term.
$\mathbf{S}_f$	surface vector.
Sc	Schmidt Number.
t	time.
T	temperature of fluid/phase k .
U_f	interface flux velocity $(\mathbf{v}_f^{(k)} \cdot \mathbf{S}_f)$.
$\mathbf{u}$	velocity vector.
u, v	velocity components in x - and y -direction, respectively.
X_{jki}	mass fraction due to coalescence between groups j and k , which goes into group i .
Y	vapor mass fraction.

GREEK SYMBOLS

α	volume fraction.
$\beta_{(k)}$	thermal expansion coefficient for phase/fluid k .
η	Kolmogorov micro-scale.
δt	time step.
ρ	density.
τ	the stress tensor.

λ	conductivity coefficient.
λ_c	coalescence efficiency.
ω_c	collision frequency.
Γ	diffusion coefficient.
ϕ	general scalar quantity.
Δh_v	latent heat.
$\Delta_P[\phi_{(k)}]$	the Δ operator.
$\mu, \mu_{turb}, \mu_{eff}$	laminar, turbulent and effective viscosity of fluid/phase k.
Ω	cell volume.
σ_1, σ_2	turbulence model constants.

SUBSCRIPTS

d	refers to the droplet discrete liquid phase.
E	refers to energy equation.
eff	refers to effective values.
g	refers to the gas phase.
i	refers to phase i.
k	refers to turbulent kinetic energy equation.
nb	refers to the east, west, ... face of a control volume.
NB	refers to the East, West, ... neighbors of the main grid point.
P	refers to the P grid point.
s	refers to the droplet surface condition.
sat	refers to the saturation condition.
ε	refers to turbulent eddy dissipation equation.
ω	refers to turbulent eddy frequency equation.
vap, g	refers to the vapor specie in the gas phase.

INTRODUCTION

This report deals with the formulation, implementation, and testing of three pressure-based numerical techniques for the prediction of mixing and evaporation of liquid fuel injected into a supersonic stream of air flowing inside a combustion chamber.

Recently there has been a revived interest in the injection of liquids in supersonic streams, particularly with respect to fuel injection techniques for hypersonic flights. These designs require air-breathing engines capable of supersonic combustion. The scramjet (supersonic combustion ramjet), appears at present to be a practical engine for these types of applications since it is capable of producing useful thrust at hypersonic speeds, using supersonic flow through the combustor. The scramjet concept itself is fairly old, and was the subject of studies throughout the 1960s and again in the 1980s. However, its coming to fruition depends among other things on the development of numerical tools for the simulation of its supersonic combustion process and related phenomena. More specifically effective penetration and enhanced mixing of hydrocarbon fuels in a gas flowing at supersonic speed is a crucial ingredient for the success of any scramjet design [1]. Three key issues govern the performance of the liquid injection process in the scramjet engine, namely: the penetration of the fuel into the free-stream, the atomization of the injected fuel drops, and the level of fuel/air mixing [2]. It is important for the fuel to penetrate effectively into the free-stream so that the combustion process produces an even temperature distribution otherwise it will mostly occur along the surface of the combustor, causing inefficient combustor operation and increased cooling problems. Rapid atomization of the fuel is also required for efficient combustion. Increased atomization of the liquid fuel results in increased fuel/air mixing which allows a higher percentage of the fuel to be burnt in the short time before the entire mixture passes out of the combustor (generally the flow residence time is of the order of few milliseconds [3]). This paper is aimed at developing three numerical methods capable of predicting the spreading and evaporation of liquid droplets injected in gases flowing at all speeds.

The complex multi-phase flow phenomenon governing liquid injection applications involves a continuous gas phase usually composed of air and the evaporating vapor species from the fuel and one or more dispersed liquid phases. Moreover, the phenomenon also entails turbulent effects. Approaches for the simulation of droplet transport and evaporation in combustion systems can be classified under two categories, namely the Lagrangian and Eulerian methods. Within both methods the gaseous phase is calculated by solving the Navier-Stokes equations with a standard discretization method such as the Finite Volume Method.

In the **Lagrangian** approach [4,5,6], the spray is represented by discrete droplets which are advected explicitly through the computational domain while accounting for evaporation and other phenomena. Due to the large number of droplets in a spray, each discrete computational droplet is made to represent a number of physical droplets averaging their characteristics. The equations of motion of each droplet are a set of ordinary differential equations (ODE) which are solved using an ODE solver, a numerical procedure different from that of the continuous phase. To account for the interaction between the gaseous phase and the spray, several iterations of alternating solutions of the gaseous phase and the spray have to be conducted. Therefore, the computational effort for strongly interacting two-phase flows with the Lagrangian method is rather large. Furthermore, for turbulent flow simulation the above model has to be augmented with a stochastic or Monte-Carlo approach.

In the **Eulerian** approach [5,6,7,8], the evaporating spray is treated as an interacting and interpenetrating continuum, in analogy to the continuum approach of single phase flows, each phase is described by a set of transport equations for mass, momentum and energy extended by interfacial exchange terms. This description allows the gaseous phase and the spray to be discretized by the same method, and therefore to be solved by the same numerical procedure. Because of the presence of multiple phases a multiphase algorithm is used rather than a single-phase one.

In this work, the numerical foundations for the simulation of supersonic droplet evaporation and scattering are developed. This is achieved by following a Eulerian-Eulerian approach using:

- 1- the full multiphase flow model,
- 2- the Multi-Size-Group model (MUSIG), and
- 3- the Heterogeneous Multi-Size-Group model (H-MUSIG).

The three approaches are implemented within an all speed pressure-based finite volume flow solver in which a droplet evaporation model is implemented. The $k-\epsilon$ [9] two-equation turbulence model has been used to account for the droplet-gas turbulence with modifications for supersonic flows. Droplet turbulence is estimated using an algebraic model based on the Boussinesq approach [7,10,11]. Different droplet sizes are considered and droplet breakup and coalescence [12,13] are modeled and their effects incorporated into the conservation equations via source terms. The use of an Eulerian approach has many advantages: same validated numerical procedure used for all phases, ease of implementation of acceleration techniques, and improvements to code can be carried over to all phases.

In the remainder of this document, the governing conservation equations for both gas and liquid droplet phases and their discretization procedure are first presented. This is followed by a detailed description of the three solution methodologies. The resulting algorithms are used to solve three physical configurations: (i) streamwise injection into a subsonic and supersonic stream flowing in a rectangular domain, (ii) cross-streamwise injection into a supersonic stream flowing in a rectangular domain are given, and (iii) streamwise injection into a supersonic stream flowing in a cylindrical domain. Results presented in the form of droplet and gas velocity, pressure, gas temperature, vapor mass fraction, air volume fraction, and gas turbulent viscosity fields and profiles are compared and conclusions drawn.

THE GOVERNING EQUATIONS

When describing multiphase flow phenomena it is implied that more than one phase exist within a small volume at any particular time. This view rests on the idea of time and space

averaging [14,15] and is equivalent to treating each phase as a continuum in the space under consideration, which requires choosing a proper scale with regard to the control volume used. For a multi-phase system the equations are derived over a representative element volume within which the different phases are present.

Except for the near region of the injector where the spray is dense, the volume fraction of the spray is low. In this dilute multi-phase flow regime, interaction between droplets can be neglected. Starting from the Navier-Stokes equations, instantaneous transport equations for the gas and droplet phase can be derived either by spatial, temporal, or ensemble averaging. However, these transport equations can only be used for the description of sprays in laminar gas flows. Since combustors generally operate in the turbulent regime, the system of equations is extended by introducing turbulent fluctuations of the transport quantities followed by Reynolds averaging of the equations. For the gaseous phase, the standard k- ϵ model is employed, while an algebraic model based on a Boussinesq approach approximates the turbulence terms in the droplet phase transport equations. The interacting flow fields are described by the transport equations presented next.

GAS EQUATIONS

The continuity, momentum, energy, turbulence kinetic energy, and turbulence dissipation rate equations for the gas phase, which is composed of two species namely air and vapor, in addition to the mass fraction equation of the fuel vapor in the gaseous phase, are respectively written as:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \mathbf{u}_g \rho_g) = \nabla \cdot \left(\frac{\mu_{t,g}}{Sc_{t,g}} \nabla \alpha_g \right) + \dot{M}_{vap,g} \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \mathbf{u}_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\alpha_g \nabla p + \nabla \cdot \overline{\boldsymbol{\tau}_g} + \mathbf{F}_g^B + \mathbf{F}_g^D + \dot{M}_{vap,g} \mathbf{u}_d \quad (2)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g k_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g k_g) = \nabla \cdot (\alpha_g \mu_{eff,k,g} \nabla k_g) + \alpha_g (P_k - \rho_g \epsilon_g) + S_{k,d} \quad (3)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \epsilon_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \epsilon_g) = \nabla \cdot (\alpha_g \mu_{eff,\epsilon,g} \nabla \epsilon_g) + \alpha_g \left(C_{\epsilon 1} \frac{\epsilon_g}{k_g} P_k - C_{\epsilon 2} \rho_g \frac{\epsilon_g^2}{k_g} \right) + S_{\epsilon,d} \quad (4)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g h_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g h_g) = -\nabla \cdot \dot{q}_g + \nabla \cdot \left(\frac{\mu_{turb,g}}{Pr_t} \nabla h_g \right) + S_{h,g} + \dot{M}_{vap,g} h_{vap,s} \quad (5)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g Y_{vap,g}) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g Y_{vap,g}) = \nabla \cdot (\alpha_g \Gamma_{Y_{vap,g},eff} \nabla Y_{vap,g}) + \dot{M}_{vap,g} (1 - Y_{vap,g}) \quad (6)$$

DROPLET BALANCE EQUATIONS

Droplet evaporation is simulated by means of the Uniform Temperature model [16,17]. This computationally effective droplet model is based on the assumption of a homogeneous internal temperature distribution in the droplet and phase equilibrium conditions at the surface. The analytical derivation of this model does not consider contributions to heat and mass transport through forced convection by the gas flow around the droplet. Forced convection is taken into account by means of two empirical correction factors ($m_{correction}$ and $h_{correction}$) [18].

$$\frac{\partial}{\partial t}(\alpha_{d,i} \rho_{d,i}) + \nabla \cdot (\alpha_{d,i} \rho_{d,i} \mathbf{u}_{d,i}) = \nabla \cdot \left(\frac{\mu_{turb,d,i}}{Sc_{turb,d,i}} \nabla \alpha_{d,i} \right) + \dot{M}_{d,i} \quad (7)$$

$$\frac{\partial}{\partial t}(\alpha_{d,i} \rho_{d,i} \mathbf{u}_{d,i}) + \nabla \cdot (\alpha_{d,i} \rho_{d,i} \mathbf{u}_{d,i} \mathbf{u}_{d,i}) = -\alpha_{d,i} \nabla p + \mathbf{F}_i^B + \mathbf{F}_i^D + \dot{M}_{d,i} \mathbf{u}_{d,i} \quad (8)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_{d,i} \rho_{d,i} h_{d,i}) + \nabla \cdot (\alpha_{d,i} \rho_{d,i} \mathbf{u}_{d,i} h_{d,i}) = & \nabla \cdot \left(\alpha_{d,i} \frac{\mu_{turb,d,i}}{Pr_{turb,d,i}} \nabla h_{d,i} \right) + \\ & h_{d,i} \nabla \cdot \left(\frac{\mu_{turb,d,i}}{Sc_{turb,d,i}} \nabla \alpha_{d,i} \right) + \pi D_i^2 \beta^* (T_g - T_{d,i}) + \dot{M}_{d,i} (\Delta h_v + h_{d,i}) \end{aligned} \quad (9)$$

where

$$\sum_i \dot{M}_{d,i} = -\dot{M}_{vap} = -\sum_i \frac{6\alpha_{d,i}}{\pi d_i^3} \dot{m}_{vap,i}^* \quad (10)$$

$$\dot{m}_{vap,i}^* = m_{correction,i} \dot{m}_{vap,i} \quad (11)$$

$$\dot{Q}_{cond,s,i}^* = \pi d_i^2 \alpha_i^* (T_{d,i} - T_g) \quad (12)$$

$$\dot{H}_{vap,s,i}^* = \dot{m}_{vap,i}^* c_{p,vap,ref,i} (T_{d,i} - T_g) \quad (13)$$

$$\dot{m}_{vap,i} = 2\pi d_i \rho_{g,ref,i} \Gamma_{im,ref,i} \ln \frac{1 - Y_{vap,g,i}}{1 - Y_{vap,s,i}} \quad (14)$$

$$\beta_i^* = h_{correction,i} \frac{\frac{\dot{m}_{vap,i} c_{p,vap,ref,i}}{\pi d_i^2}}{\exp\left(\frac{\dot{m}_{vap,i} c_{p,vap,ref,i}}{2\pi d_i \lambda_{g,ref,i}}\right) - 1} \quad (15)$$

$$m_{correction,i} = 1 + 0.276 \text{Re}_{d,i}^{1/2} \text{Sc}_i^{1/3} \quad (16)$$

$$h_{correction,i} = 1 + 0.276 \text{Re}_{d,i}^{1/2} \text{Pr}_i^{1/3} \quad (17)$$

$$\mu_{turb,d,i} = \mu_{turb,g} \frac{\rho_{d,i}}{\rho_g} \frac{k_{d,i}}{k_g} \quad (18)$$

For an N-phase flow, the volume fractions $\alpha^{(k)}$ are characterized by the condition:

$$\sum_{k=1}^N \alpha^{(k)} = 1 \quad (19)$$

The ratio of the turbulent kinetic energies of a dispersed (d) and gas (g) phase is calculated following the approach in [7,11]:

$$\frac{k_d}{k_g} = \frac{1}{1 + \omega^2 \tau^2} \quad (20)$$

where

$$k_d = \frac{1}{2} \mathbf{u}'_d \cdot \mathbf{u}'_d \quad (21)$$

Since in general the droplets do not follow the motion of the surrounding fluid from one point to another it is expected for the ratio k_d / k_g to be different from unity and varies with particle relaxation time τ and local turbulence quantities. Krämer [11] recommends the following equation for the frequency of the particle response:

$$\omega = \frac{1}{\tau} \left(\frac{\sqrt{\frac{2}{3}} k_g}{L_x} \tau \right)^{1/4} \quad (22)$$

$$\tau = \frac{1}{18} \frac{\rho_d}{\rho_g} \frac{D^2}{\nu} \frac{1}{1 + 0.133 \text{Re}_d^{0.687}}$$

with a characteristic macroscopic length scale of turbulence given by

$$L_x = \left(c_\mu \right)^{3/4} \frac{\left(k_g \right)^{3/2}}{\epsilon_g} \quad (23)$$

DISCRETIZATION PROCEDURE

A review of the above differential equations reveals that they are similar in structure. If a typical representative variable associated with phase (k) is denoted by $\phi^{(k)}$, the general fluidic differential equation may be written as:

$$\frac{\partial(\alpha^{(k)}\rho^{(k)}\phi^{(k)})}{\partial t} + \nabla \cdot (\alpha^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}) = \nabla \cdot (\alpha^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}) + \alpha^{(k)}Q^{(k)} \quad (24)$$

where the expression for $\Gamma^{(k)}$ and $Q^{(k)}$ can be deduced from the parent equations.

The general conservation equation (24) is integrated over a finite volume to yield:

$$\iint_{\Omega} \frac{\partial(\alpha^{(k)}\rho^{(k)}\phi^{(k)})}{\partial t} d\Omega + \iint_{\Omega} \nabla \cdot (\alpha^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}) d\Omega = \iint_{\Omega} \nabla \cdot (\alpha^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}) d\Omega + \iint_{\Omega} \alpha^{(k)}Q^{(k)} d\Omega \quad (25)$$

Where Ω is the volume of the control cell. Using the divergence theorem to transform the volume integral into a surface integral, replacing the surface integrals by a summation of the fluxes over the sides of the control volume, and then discretizing these fluxes using suitable interpolation profiles the following algebraic equation results:

$$A_p^{(k)}\phi_p^{(k)} = \sum_{NB} A_{NB}^{(k)}\phi_{NB}^{(k)} + B_p^{(k)} \quad (26)$$

In compact form, the above equation can be written as

$$\phi^{(k)} = H_p[\phi^{(k)}] = \frac{\sum_{NB} A_{NB}^{(k)}\phi_{NB}^{(k)} + B_p^{(k)}}{A_p^{(k)}} \quad (27)$$

An equation similar to equation (26) is obtained at each grid point in the domain and the collection of these equations forms a system that is solved iteratively.

The discretization procedure for the momentum equation yields an algebraic equation of the form:

$$\mathbf{u}_p^{(k)} = \mathbf{H}_p[\mathbf{u}^{(k)}] - \alpha^{(k)}\mathbf{D}_p^{(k)}\nabla_p(P) \quad (28)$$

Furthermore, the phasic mass-conservation equation can be viewed as a phasic volume fraction equation, which can be written as:

$$\alpha_p^{(k)} = H_p[\alpha^{(k)}] \quad (29)$$

or as a phasic continuity equation to be used in deriving the pressure correction equation:

$$\frac{(\alpha_p^{(k)}\rho_p^{(k)}) - (\alpha_p^{(k)}\rho_p^{(k)})^{Old}}{\delta t} \Omega + \Delta_p[\alpha^{(k)}\rho^{(k)}\mathbf{u}^{(k)} \cdot \mathbf{S}] = \alpha^{(k)}\dot{M}^{(k)} \quad (30)$$

where the Δ operator represents the following operation:

$$\Delta_P[\Theta] = \sum_{f=nb(P)} \Theta_f \quad (31)$$

PRESSURE CORRECTION EQUATION

To derive the pressure-correction equation, the mass conservation equations of the various fluids are added to yield the global mass conservation equation given by:

$$\sum_k \left\{ \frac{(\alpha_p^{(k)} \rho_p^{(k)}) - (\alpha_p^{(k)} \rho_p^{(k)})^{Old}}{\delta t} \Omega + \Delta_p (\alpha^{(k)} \rho_p^{(k)} \mathbf{u}^{(k)} \cdot \mathbf{S}) \right\} = 0 \quad (32)$$

Denoting the corrections for pressure, density, and velocity by P' , $\mathbf{u}^{(k)'}$, and $\rho^{(k)'}$, respectively, the corrected fields are written as:

$$P = P^\circ + P', \mathbf{u}^{(k)} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, \rho^{(k)} = \rho^{(k)\circ} + \rho^{(k)'} \quad (33)$$

Combining equations (28), (32), and (33), the final form of the pressure-correction equation is obtained as [19]:

$$\begin{aligned} \sum_k \left\{ \frac{\Omega}{\delta t} r_p^{(k)\circ} C_\rho^{(k)} P'_p + \Delta_p [r^{(k)\circ} U^{(k)*} C_\rho^{(k)} P'] - \Delta_p [r^{(k)\circ} \rho^{(k)*} (r^{(k)\circ} \mathbf{D}^{(k)} \nabla P') \cdot \mathbf{S}] \right\} \\ = - \sum_k \left\{ \frac{r_p^{(k)\circ} \rho_p^{(k)*} - (r_p^{(k)} \rho_p^{(k)})^{old}}{\delta t} \Omega + \Delta_p [r^{(k)\circ} \rho^{(k)*} U^{(k)*}] \right\} \end{aligned} \quad (34)$$

The corrections are then applied to the velocity, density, and pressure fields using the following equations:

$$\mathbf{u}_p^{(k)*} = \mathbf{u}_p^{(k)\circ} - r^{(k)\circ} \mathbf{D}_p^{(k)} \nabla_p P', \quad P^* = P^\circ + P', \quad \rho^{(k)*} = \rho^{(k)\circ} + C_\rho^{(k)} P' \quad (35)$$

THE MULTIPHASE FLOW MODEL

In the multiphase model, displayed schematically in Figure 1, the dispersed phase is subdivided into N size group classes where each class is treated as a continuum phase in the calculation. Although this model can describe a real multi-phase flow problem however the number of coupled equations associated with this model is very large. The number of size groups should therefore be limited to low values due to the extensive numerical effort of the coupled equations.

In order to keep track of the droplet size, an additional diameter equation is solved for every droplet phase. This equation is derived based on mass conservation and is given by

$$\frac{\partial}{\partial t}(\alpha_{d,i}\rho_{d,i}d_i) + \nabla \cdot (\alpha_{d,i}\mathbf{u}_{d,i}\rho_{d,i}d_i) = \nabla \cdot \left(\alpha_{d,i} \frac{\mu_{turb,d,i}}{\text{Pr}_{turb,d,i}} \nabla d_i \right) + d_i \nabla \cdot \left(\frac{\mu_{turb,d,i}}{\text{Sc}_{turb,d,i}} \nabla \alpha_{d,i} \right) + \frac{4}{3}d_i \dot{M}_{d,i} \quad (36)$$

This multi-phase model, is an extension of the work performed in [20]. Results generated using this model are the baseline against which results generated using the MUSIG and H-MUSIG models are compared.

FULL MULTIPHASE SOLUTION PROCEDURE

The overall solution procedure is an extension of the single-phase SIMPLE algorithm [21,22] into multi-phase flows [19]. The sequence of events in the MCBA-SIMPLE is as follows:

1. Solve the fluidic momentum equations for velocities.
2. Solve the pressure correction equation based on global mass conservation.
3. Correct velocities, densities, and pressure.
4. Solve the fluidic mass conservation equations for volume fractions.
5. Solve the fluidic scalar equations (k , ϵ , T , Y , D , etc...).
6. Return to the first step and repeat until convergence.

THE MULTI-SIZE-GROUP MODEL (MUSIG)

The MUSIG (MUltiple-SIze-Group) model [23,24] represents a further development of the multiphase model outlined above. The MUSIG model was originally developed for the prediction of bubbles in water and has never been used for the prediction of mixing and evaporation of liquid droplets in a stream of gas. It is the intention of this work to extend the applicability of MUSIG to such configuration.

As a first step for describing the MUSIG model, an explanation of the population balance approach is provided. This is followed by the model description, the equations involved, and the break up and coalescence models used.

POPULATION BALANCE APPROACH

In spray modeling, a wide range of particle sizes and shapes exist at every point in the dispersed phase, which makes the description of the size and shape of the droplets very difficult. This difficulty is further magnified when break up and coalescence occur due to their great influence on the overall performance among the phases. Therefore it is essential in modeling spray flows to use a formulation that take into account the different size distribution of particles in addition to the birth and death processes that may be encountered [25]. This is accomplished through the use of the population balance approach.

The formulation of the population balance could be either based on the Boltzmann transport equation or on continuum mechanics [26]. It represents the transport of the number density of the fluid through the space taking into account birth and death of particles due to breakup and coalescence. The fluid particle number density transport equations of particles having volume v_i , i.e. group size i , is given as follows:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{u} n_i) = S_i + (S_{ph})_i \quad (37)$$

The interaction term S_i represents the net rate of change in the number density distribution function, n_i , due to particle break-up and coalescence; in other words this term accounts for both the birth of particles of size i (due to either breakup of larger particles or coalescence of smaller ones) and death of particles of size i (also due to breakup and coalescence but this time of particles of size i which goes into other groups). A general representation of these source and sink terms is given as

$$S_i = B_{Bi} - D_{Bi} + B_{Ci} - D_{Ci} \quad (38)$$

Moreover the term S_{ph} is added to the population balance equation (Eq. (37)) in order to account for phase change since size change can occur because of birth due to nucleation, condensation and evaporation [27].

MUSIG MODEL DESCRIPTION

In this model, displayed schematically in Figure 2, the dispersed phase is decomposed into N size groups chosen according to the problem at hand (say $N=10$) where all groups are treated as one continuum phase thus moving at the same speed and N continuity or population balance equations are solved. The single disperse phase is thus characterized by various size

groups, from which a local Sauter mean diameter is deduced. An accurate determination of the droplet Sauter diameter is crucial in order to calculate the interfacial area based on which the interphase heat and mass transfer and momentum drags could be evaluated.

A discretization is performed in order to evaluate the diameter (d_i) of each size group. Any of the following three approaches can be used [24]: (a) the equal mass discretization, (b) the equal diameter discretization, (c) The geometric mass discretization. In all three methods the minimum and maximum diameters of the polydispersed fluid are set before beginning the calculations.

MUSIG MODEL FORMULATION

As described previously a continuity equation for each size group (a population balance equation) is solved, but it is assumed that all droplets move with the same velocity so that only one set of momentum equations for the dispersed phase has to be solved.

let f_i be the size fraction of the polydispersed phase which appears in group size i , ρ_d the density of the dispersed phase, if Equation (38) is multiplied by m_i , it reduces to the following:

$$\begin{aligned} \rho_d &= \frac{m_i}{\Omega_i} \quad \& \quad \alpha_i = n_i \Omega_i \\ \alpha_i &= \alpha_d f_i \\ \frac{\partial}{\partial t} (\rho_d \alpha_d f_i) + \nabla \cdot (\rho_d \alpha_d f_i \mathbf{u}_i) &= S_i + (S_{ph})_i \end{aligned} \tag{39}$$

Since this model assumes that all particles have the same velocity, u_i is replaced by u_d (velocity of the dispersed phase) and the above equation reduces to

$$\frac{\partial}{\partial t} (\rho_d \alpha_d f_i) + \nabla \cdot (\rho_d \alpha_d f_i \mathbf{u}_d) = S_i + (S_{ph})_i \tag{40}$$

This equation has the form of the transport equation of a scalar variable f_i , in the dispersed phase in which the source term S_i accounts for the birth of droplets of size i due to breakup of droplets of larger size and coalescence of droplets of smaller size which go into i and death of droplets of size i due to both break up and coalescence encountered in this size group. Therefore the sum of this term over all size groups is equal to zero

$$\sum_i S_i = 0 \tag{41}$$

If summation over all size groups is performed, an overall continuity equation for the dispersed phase is derived. Performing this summation and noticing that $\sum_{i=1,N} f_i = 1$, the overall continuity equation for the dispersed phase is found as

$$\begin{aligned}
 & \frac{\partial}{\partial t}(\rho_d \alpha_d f_1) + \nabla \cdot (\rho_d \alpha_d f_1 \mathbf{u}_d) = S_1 - f_1 \dot{M}_{vap,g} \\
 & \frac{\partial}{\partial t}(\rho_d \alpha_d f_2) + \nabla \cdot (\rho_d \alpha_d f_2 \mathbf{u}_d) = S_2 - f_2 \dot{M}_{vap,g} \\
 & + \quad \quad \quad \vdots \\
 & \quad \quad \quad \vdots \\
 & \quad \quad \quad \vdots \\
 & \frac{\partial}{\partial t}(\rho_d \alpha_d f_N) + \nabla \cdot (\rho_d \alpha_d f_N \mathbf{u}_d) = S_N - f_N \dot{M}_{vap,g}
 \end{aligned} \tag{42}$$

$$\frac{\partial}{\partial t}(\rho_d \alpha_d) + \nabla \cdot (\rho_d \alpha_d \mathbf{u}_d) = -\dot{M}_{vap,g}$$

The continuity equation is therefore used to solve the population balance equations with the source term to be connected with the source of population balance equations. It is important to note here that no extra scalar equations are needed for the population balance equation [28].

After solving the population balance equations, the droplet sauter diameter which represents an average representation of the dispersed phase is calculated, and the dispersed phase calculations are then performed assuming the monodispersed phase with the diameter of the phase being equal to the local droplet Sauter diameter d_s based on the values of the size fractions of the dispersed phase f_i and discrete droplet sizes d_i given by:

$$\frac{1}{d_s} = \sum_{i=1}^N \left(\frac{f_i}{d_i} \right) \tag{43}$$

As in the multi-phase model, a continuity equation for each size group is solved, but it is assumed that all droplet velocities can be related to the average value in an algebraic manner, so that only one set of momentum equations for the gas phase is solved. This single disperse phase is characterized by various size groups, from which a local Sauter mean diameter is deduced. An accurate determination of the droplet Sauter diameter is crucial in order to calculate the interfacial area based on which the interphase heat and mass transfer and momentum drags could be evaluated.

The MUSIG model essentially reduces the multiphase approach described above back to a two-fluid approach with one velocity field for the continuous phase and one for the dispersed phase. However, the continuity equations of the particle size groups are retained and solved to represent the size distribution. With this approach, it is possible to consider a larger number of particle size groups (say 10, 20 or even 30 particle phases) to give a better representation of the size distribution.

BREAK UP AND COALESCENCE MODELS

Various models have been implemented for the calculation of the break-up and coalescence rates. The overall form of these models is similar, with different correlations used for coalescence and break-up depending on the nature of the flow [27].

The specific models that has been implemented for the break-up and coalescence rates are due to Luo and Svendsen [12] and Coulaloglou and Tavlarides [13].

LUO AND SVENDSEN BREAKUP MODEL

The net source to group i due to breakup (using any break up model) is:

$$B_{Bi} - D_{Bi} = \rho_d \alpha_d \left(\sum_{j>i} B_{ji} f_j - f_i \sum_{j<i} B_{ij} \right) \quad (44)$$

The break-up rate B_{ij} is assumed to be a function of the break-up fraction B'_{ij} as follows:

$$B_{ij} = B'_{ij} \int_{f_{BV}} d f_{BV} \quad (45)$$

This model is based on the following five main assumptions:

- 1- The turbulence is assumed to be isotropic.
- 2- Binary breakage of fluid particles is only considered (turbulent breakage and Shear breakage). The breakage volume fraction is assumed to be given by

$$f_{BV} = \frac{m_i}{m_j} = \frac{d_i^3}{d_j^3} \quad (46)$$

Where d_j is the diameter of a mother particle splitting into two particles of sizes d_i and $(d_j^3 - d_i^3)^{1/3}$.

- 3- The occurrence of breakup is determined by the energy level of the arriving eddy. The particle oscillation frequency is larger than the arrival frequency of eddies. This implies that eddies affect the particles independently in a way that once an eddy of sufficiently high energy arrives, the particle will break.
- 4- Eddies of size scale smaller than or equal to the particle diameter induce particle oscillation and dominate the deformation of the particles in the flow field while larger eddies are responsible for the translatory motion of particles.

The break-up frequency of a mother particle with size d_j splitting into two particles of sizes d_i and $(d_j^3 - d_i^3)^{1/3}$ is given by:

$$B'_{ji} = 0.923 F_B (1 - \alpha_d) \left(\frac{\varepsilon_c}{d_j^2} \right)^{1/3} \underbrace{\int_{\xi_{\min}}^{\infty} \frac{(1 + \xi)^2}{\xi^{11/3}} e^{-\frac{12\sigma(f_{BV}^{2/3} + (1 - f_{BV})^{2/3} - 1)}{\beta \rho_c \varepsilon_c^{2/3} d_j^{5/3} \xi^{11/3}}} d\xi}_I \quad (47)$$

where F_B is added as a calibration factor of the model, ε_g is the continuous phase eddy dissipation energy, σ is the surface tension, $\beta=2$, and ξ is the dimensionless size of eddies in the inertial subrange of isotropic turbulence. The lower limit of the integration is given by

$$\xi_{\min} = 11.4 \frac{\eta}{d_j} \quad (48)$$

and the Kolmogorov micro-scale η is given by:

$$\eta = \left[(\mu_c / \rho_c)^3 / \varepsilon_c \right]^{1/4} \quad (49)$$

COULALOGLOU AND TAVLARIDES COALESCENCE MODEL

Collisions may happen due to various mechanisms however this model only considers the collisions of droplets due to turbulence, buoyancy and laminar shear.

The net source to group i due to coalescence is given as

$$B_{Ci} - D_{Ci} = (\rho_d \alpha_d)^2 \left(\frac{1}{2} \sum_{j \leq i} \sum_{k \leq i} C_{jk} f_j f_k \frac{m_j + m_k}{m_j m_k} X_{jki} - \sum_j C_{ij} f_i f_j \frac{1}{m_j} \right) \quad (50)$$

where C_{ij} is the specific coalescence rate between groups i and j and X_{jki} represents the fraction of mass due to coalescence between groups j and k which goes into i and is written as

$$X_{jki} = \begin{cases} \frac{(m_j + m_k) - m_{i-1}}{m_i - m_{i-1}} & \text{if } m_{i-1} < (m_j + m_k) < m_i \\ \frac{m_{i+1} - (m_j + m_k)}{m_{i+1} - m_i} & \text{if } m_i < (m_j + m_k) < m_{i+1} \\ 1 & \text{if } m_j + m_k \geq m_{\max} = m_i \\ 0 & \text{otherwise} \end{cases} \quad (51)$$

$$\sum_i X_{jki} = 1 \quad \text{for all } j, k \quad (52)$$

When summed over all size groups, the net source due to coalescence is zero.

The coalescence rate C_{ij} of the dispersed phase drops in a turbulent flow field is described as the product of the collision frequency $\omega_c(d_i, d_j)$ and the corresponding coalescence efficiency $\lambda_c(d_i, d_j)$ as is written as

$$C_{ij} = \omega_c(d_i, d_j) \lambda_c(d_i, d_j) \quad (53)$$

In the Coulaloglou and Tavlarides [13] model it is assumed that the mechanism of collision in a locally isotropic flow field is analogous to collisions between molecules as in kinetic theory of gases, the collision frequency between two drops with volumes Ω_i and Ω_j are expressed as

$$\omega_c(d_i, d_j) = K_c \frac{\epsilon_c^{1/3}}{1 + \alpha_d} (d_i + d_j)^2 (d_i^{2/3} + d_j^{2/3})^{1/2} \quad (54)$$

The coalescence efficiency is based on the film drainage mechanism where the drops are considered to cohere together and be prevented by coalescence by a film of continuous phase trapped between them. The coalescence efficiency as suggested by Coulaloglou and

Tavlarides is given as

$$\lambda(d_i, d_j) = \exp \left[-K \frac{\mu_c \rho_c \epsilon_c}{\sigma^2 (1 + \alpha_d)^3} \left(\frac{d_i d_j}{d_i + d_j} \right)^4 \right] \quad (55)$$

MUSIG SOLUTION PROCEDURE

The overall two-phase MUSIG solution procedure is as follows:

1. Solve the fluidic momentum equations for the gas and droplet phase for velocities.
2. Solve the pressure correction equation based on global mass conservation.
3. Correct velocities, densities, and pressure.
4. Solve the fluidic mass conservation equations for droplet and air volume fractions.
5. Calculate sources due breakup and coalescence.
6. Solve the population fraction equations.
7. Calculate Sauter diameter.
8. Solve the fluidic scalar equations (k , ϵ , T , Y).
9. Return to the first step and repeat until convergence.

THE HETEROGENEOUS MUSIG MODEL (H-MUSIG)

With the MUSIG model, it is possible to consider a larger number of particle size groups to give a better representation of the size distribution. The shortcoming of this approach however [29, 30], is related to the droplet groups common velocity. It is well known that larger droplets do not follow the flow and smaller droplets do. By considering one average velocity for the droplets, a stratification of droplet sizes from normal fuel injection occurs with larger droplets penetrating further into the flow. The larger droplets transport more fuel mass than may be expected. To alleviate this problem, it is proposed to extend the (homogeneous) MUSIG model into a Multi-phase MUSIG model or a Heterogeneous MUSIG model (H-MUSIG). In the extended model, rather than assigning one velocity for all droplet groups, classes of groups will be considered with droplet groups in a class sharing the same velocity. This suggested approach, displayed schematically in Figure 3, could be seen as a blend between a full multi-phase approach and a two-phase approach. If a group is composed of one droplet class, then the full multi-phase approach is obtained, whereas if a group is composed of all droplet sizes, then the original MUSIG is recovered.

H-MUSIG MODEL DESCRIPTION

In this model, the dispersed phase is divided into N fields, each allowing an arbitrary number of sub-size classes [29,30]. Therefore N velocity fields are to be solved where each field is subdivided into M_l size groups moving at the same mean algebraic velocity. M_l population fraction equations need to be solved along with one set of momentum equations for each field.

The sub-size groups are discretized in order to evaluate the diameter (d_i) of each size group. The droplet average diameter for each sub-size class is calculated using one of the group size algorithms described above. The lower and upper boundaries for each field should be set in order for the average diameter to be calculated.

H-MUSIG MODEL FORMULATION

As described earlier, a continuity or a population balance equation for each sub-size group is solved. Let $l, l \in [1, N]$ be a group field number; the volume fractions of sub-classes, groups and the dispersed phase are related as follows:

$$\alpha_i = \alpha_d f_i = \alpha_{F_l} f_{F_l,i} \quad (56)$$

where f_i is the size fraction of the polydispersed phase which appears in group sub-size i , $f_{l,i}$ is the population fraction of sub-group size i in the field l , ρ_d the density of the dispersed phase, α_i is the volume fraction of sub-group size i and α_{F_l} is the volume fraction of field l . If Eq. (40) is multiplied by m_i , the population fraction equation for each sub-size group in class field l reduces to

$$\frac{\partial}{\partial t} (\rho_d \alpha_{F_l} f_{F_l,i}) + \nabla \cdot (\rho_d \alpha_{F_l} f_{F_l,i} \mathbf{u}_{F_l}) = S_{F_l,i} + \frac{\alpha_{F_l}}{\alpha_d} f_{F_l,i} S_{ph} \quad (57)$$

Summing over all sub-classes in field l and applying the following additional relations

$$S_{F_l} = \sum_{i=1}^{M_{F_l}} S_{F_l,i} \quad \sum_{i=1}^{M_{F_l}} \frac{\alpha_{F_l}}{\alpha_d} f_{F_l,i} = \frac{\alpha_{F_l}}{\alpha_d} \quad (58)$$

The continuity equation for each field or the volume fraction equation is found as

$$\frac{\partial}{\partial t} (\rho_d \alpha_{F_l}) + \nabla \cdot (\rho_d \alpha_{F_l} \mathbf{u}_{F_l}) = S_{F_l} + \frac{\alpha_{F_l}}{\alpha_d} S_{ph} \quad (59)$$

Additional relations and constraints are further added to this model:

$$\alpha_d = \sum_{l=1}^N \alpha_{F_l} = \sum_{i=1}^{N \times M} \alpha_i \quad \sum_{i=1}^{M_{F_l}} f_{F_l,i} = 1 \quad \sum_{i=1}^{N \times M} f_i = 1 \quad (60)$$

The source $S_{F_l,i}$ is the net rate at which mass accumulates in sub-size group i due to coalescence of particles of smaller size than i in all field and breakup of particles of larger sizes than i in all fields. Mathematicall $S_{F_l,i}$ is given by

$$S_{F_l,i} = B_{i,B} - D_{i,B} + B_{i,C} - D_{i,C} \quad (61)$$

Here the birth and death rates are treated using specific breakup and coalescence models since they represents rates in the dispersed phase for all sub-classes with

$$S_{F_l} = \sum_{i=1}^{M_{F_l}} S_{F_l,i} \quad \& \quad \sum_{l=1}^N S_{F_l} = 0 \quad (62)$$

The overall continuity of the dispersed phase is derived by summing over all groups using the above mentioned relation and is found to be

$$\frac{\partial}{\partial t} (\rho_d \alpha_d) + \nabla \cdot (\rho_d \alpha_d \mathbf{u}_{F_l}) = S_{ph} \quad (63)$$

After solving the population balance equations for each sub-size group, the droplet sauter diameter that represents an average representation of the dispersed phase field l is calculated, and the phase field calculations are then performed assuming the monodispersed phase for each field with the diameter of the phase field being equal to

$$d_{s,F_l} = \frac{1}{\sum_{i=1}^{M_{F_l}} \frac{f_{F_l,i}}{d_i}} \quad (64)$$

For each field, the momentum equation that need to be solved (since the velocities differ) is given by

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_d \alpha_{F_l} \mathbf{u}_{F_l}) + \nabla \cdot (\rho_d \alpha_{F_l} \mathbf{u}_{F_l} \mathbf{u}_{F_l}) = & -\alpha_{F_l} \nabla P + \\ & \nabla \cdot \alpha_{F_l} \mu_{urb,d} (\nabla u_{F_l} + \nabla u_{F_l}^T) + \alpha_{F_l} \rho_d g + F_{F_l} + M_{F_l} + S_{M_{F_l}} \end{aligned} \quad (65)$$

where M_{F_l} is the source term associated with momentum due to phase change, F_{F_l} is the momentum transfer between the dispersed field l phase and the continuous phase, and $S_{M_{F_l}}$ is

the source term due to the transfer of momentum between different velocity groups due to breakup and coalescence processes leading to the formation of particles belonging to other groups.

H-MUSIG MODEL SOLUTION STRATEGY

The solution algorithm of the system is as follows:

1. The momentum equations for all phases are solved in order to calculate the velocities of the different phase fields and the continuous phase.
2. The Global continuity equation derived by summing continuity for all phases is then solved to calculate the pressure, which is the same for all phases.
3. The continuity equations or volume fraction equations are then solved to calculate the volume fraction of the dispersed phases (note that the volume fraction equations of the various phase fields include a source term due to particles break up and coalescence).
4. Calculate sources due breakup and coalescence.
5. Solve the population fraction equations for the groups of each droplet phase.
6. Calculate Sauter diameters of the various phases.
7. Solve the fluidic scalar equations for all phases (k , ϵ , T , Y).
8. Return to the first step and repeat until convergence.

COMPARISON BETWEEN MUSIG AND H-MUSIG

A summary of the differences between MUSIG and H-MUSIG is shown in the table below.

Table 1 Comparison between homogeneous and inhomogeneous model

H-MUSIG	MUSIG
Dispersed phase accounts for N phase fields or classes	Dispersed phase accounts for one phase field or class
Each class is subdivided into M groups	The class is divided into N groups
N sets of momentum equations needs to be solved	1 set of momentum equations needs to be solved
Source term due to break up and coalescence resulting in the birth or death of particle of size i in the population balance equations is the same	
The volume fraction equation for each class l includes a source term associated with the particle break up and coalescence contributions (term S_{F_l})	No Contributions for particle breakup and coalescence in the volume fraction equation since no other dispersed class is present
Interphase momentum and energy transfer term due to the presence of various velocity and energy fields are added to the momentum and energy equations, respectively.	

RESULTS AND DISCUSSION

In what follows, solutions to three two-dimensional multi-phase flow problems are presented and discussed. The physical situations for these problems are displayed in Figure 4. Figure 4(a) represents a rectangular duct in which air enters with a uniform free stream velocity U , while fuel (Kerosene is used in all computations due to the unavailability of the physical properties of JP-7 fuel to the author) mixed with air is injected through a nozzle 2 mm in diameter in the stream-wise direction through 120° angle. Figure 4(b) is similar to Figure 4(a)

with the exception of the domain being cylindrical (axi-symmetric) and as such only half the cylindrical enclosure is considered. Figure 4(c) represents the same rectangular duct displayed in Figure 4(a) with fuel being injected in the cross-stream direction. The length of the domain is L and its width is W ($W=L/4$). Turbulent flow results are generated using the $k-\epsilon$ turbulence models. Solutions for the above configurations are generated using the various methodology and results are compared.

STREAMWISE INJECTION IN A RECTANGULAR DOMAIN

The physical domain depicted in Fig. 4(a) is subdivided into 120×102 non-uniform control volumes. The length L of the domain is 1 m. The fuel is injected with a velocity of magnitude 30 m/s through 12 uniform control volumes (each of width $.001/12$ m) at different injection angles (varying uniformly from -60° to 60° as shown in Fig. 4(a)). In order to show the applicability of the solutions procedures for fluid flowing at all speeds, results for this configuration are generated for fuel injection in both subsonic and supersonic streams.

Evaporation and mixing of fuel droplets in a subsonic stream

For the physical situation depicted in Fig. 4(a), the Mach number and temperature of the air at inlet to the domain are taken to be 0.2 ($M_{\text{air,inlet}}=0.2$) and 700 K, respectively. The mixture of air and droplets are injected into the domain with a temperature of 350 K with the volume fraction of Kerosene in the injected air-fuel mixture being 0.1. The velocity of the injected mixture is set at 30 m/s with the angle of injection varying from -60° to 60° . With this velocity profile and volume fraction a total of 1.8327 Kg/s/m of fuel are injected into the domain.

Full multiphase results are generated using 5 droplet phases of sizes of $60\ \mu\text{m}$, $80\ \mu\text{m}$, $100\ \mu\text{m}$, $120\ \mu\text{m}$, and $140\ \mu\text{m}$ with their inlet volume fractions being 0.0125, 0.0225, 0.03, 0.0225, and 0.0125 respectively. For the MUSIG model, the droplet phase is divided into 10 groups using the equal diameter discretization with the diameter of the smallest droplet set to $55\ \mu\text{m}$ and the increment to $10\ \mu\text{m}$ with population fractions of 0.05, 0.075, 0.1, 0.125, 0.15, 0.15, 0.125, 0.1, 0.075, and 0.05, respectively. For the H-MUSIG model, two droplet phases are

considered, each divided into five group sizes discretized using the equal diameter discretization. The diameters and population fractions of the various groups are similar to those used with MUSIG. An important parameter for comparison is the percent of the injected fuel that has evaporated into the gas field. These percentages are found to be 30.83%, 27.78%, and 27.27% for the full multiphase method, the H-MUSIG model, and the MUSIG model respectively.

Comparison of results obtained using the various techniques are presented in Figures 5 through 10. Figure 5 displays the velocity fields for some of the droplet phases. Figure 5(a)-5(c) depicts the velocity vectors for droplet phases 1 (60 μm in diameter), 3 (100 μm in diameter), and 5 (140 μm in diameter) using the full multiphase approach. H-MUSIG droplet velocity vectors are presented in Figures 5(d) and 5(e), while Figure 5(f) shows the droplet vector field predicted using MUSIG. Both the multiphase and the H-MUSIG results reveal a larger droplet penetration with increasing droplet diameter, which is physically correct as larger particles possess higher inertia and are more capable of penetrating into the domain as compared to smaller ones, which align faster with the flow field. Further the path of the droplets predicted by MUSIG is between the trajectories of the smaller and larger droplet phases predicted by H-MUSIG (Compare Fig. 5(f) against Figures 5(d) and 5(e)). The same is true for H-MUSIG and the full multiphase results (compare Figure 5(d) against Figures 5(a) and 5(b); and Figure 5(e) against Figures 5(b) and 5(c)).

Comparisons in the form of contour maps of the gas phase volume fraction, vapor mass fraction, pressure field, and gas temperature fields generated by the various methods are depicted in Figures 6, 7, 8, and 9 respectively. As can be seen, the overall structure of the various fields are similar even though there exist some variations in the details. The volume fraction fields (Figure 6) reflect the droplet velocity fields displayed in Figure 5, with the droplet volume fraction decreasing as droplets move in the domain. As expected, the vapor mass fraction (Figure 7) in the gas phase maximizes at exit from the domain with the full multiphase results showing less evaporation in the region around the centerline of the domain. Pressure and temperature field maps presented in Figures 8 and 9 show similar profiles with

slight variation in levels. This is further revealed in the comparison of profiles presented in Figure 10. In this figure, u-velocity, gas temperature, pressure, and vapor mass fraction profiles across the domain at $x=0.5$ generated using the various algorithms are compared. The gas u-velocity profiles (Figure 10(a)) obtained by the various methods are nearly coincident. The temperature profiles however (Figure 10(b)), show some differences in the region around the centerline of the domain, with H-MUSIG predicting the lowest gas temperature. This is in line with the vapor mass fraction contours presented earlier and the vapor mass fraction profiles in Figure 10(d), which reveal higher vapor mass fraction around the centerline predicted by H-MUSIG and consequently lower gas temperature. Moreover, profiles in Figure 10(d) show that full multiphase results are close to H-MUSIG results in area away from the centerline and are close to MUSIG results in the region around the centerline. Pressure profiles presented in figure 10(c) indicate lower level values with the full multiphase approach. Values obtained by MUSIG and H-MUSIG are very close.

Evaporation and mixing of fuel droplets in a supersonic stream

For the physical situation depicted in Fig. 4(a), the Mach number and temperature of the air at inlet to the domain are taken to be 2 ($M_{\text{air,inlet}}=2$) and 700 K, respectively. The mixture of air and droplets are injected into the domain with a temperature of 350 K with the volume fraction of Kerosene in the injected air-fuel mixture being 0.1. The velocity of the injected mixture is set at 30 m/s with the angle of injection varying from -60° to 60° . With this velocity profile and volume fraction a total of 1.8327 Kg/s/m of fuel are injected into the domain.

Full multiphase results are generated using 5 droplet phases of sizes of $60\mu\text{m}$, $80\mu\text{m}$, $100\mu\text{m}$, $120\mu\text{m}$, and $140\mu\text{m}$ with their inlet volume fractions being 0.0125, 0.0225, 0.03, 0.0225, and 0.0125 respectively. For the MUSIG model, the droplet phase is divided into 10 groups using the equal diameter discretization with the diameter of the smallest droplet set to $55\mu\text{m}$ and the increment to $10\mu\text{m}$ with population fractions of 0.05, 0.075, 0.1, 0.125, 0.15, 0.15, 0.125, 0.1, 0.075, and 0.05, respectively. For the H-MUSIG model, two droplet phases are

considered, each divided into five group sizes discretized using the equal diameter discretization. The diameters and population fractions of the various groups are similar to those used with MUSIG. An important parameter for comparison is the the percent of the injected fuel that has evaporated in the domain. These percentages are found to be 9.69%, 12%, and 12.38% for the full multiphase method, the H-MUSIG model, and the MUSIG model respectively.

Comparison of results obtained using the various techniques are presented in Figures 11 through 16. Figure 11 displays the velocity fields for some of the droplet phases. Figure 11(a)-11(c) depicts the velocity vectors for droplet phases 1 (60 μm in diameter), 3 (100 μm in diameter), and 5 (140 μm in diameter) using the full multiphase approach. H-MUSIG droplet velocity vectors are presented in Figures 11(d) and 11(e), while Figure 11(f) shows the droplet vector field predicted using MUSIG. Due to the small velocity by which the fuel is injected (30 m/s) as compared to the gas velocity (1061 m/s) the spread is much lower than the subsonic case. Nevertheless, both the multiphase and the H-MUSIG results reveal a larger droplet penetration with increasing droplet diameter, which is physically correct as larger particles possess higher inertia and are more capable of penetrating into the domain as compared to smaller ones, which align faster with the flow field. Further the path of the droplets predicted by MUSIG is between the trajectories of the smaller and larger droplet phases predicted by H-MUSIG (Compare Fig. 11(f) against Figures 11(d) and 11(e)). The same is true for H-MUSIG and the full multiphase results (compare Figure 11(d) against Figures 11(a) and 11(b); and Figure 11(e) against Figures 11(b) and 11(c)).

Comparisons in the form of contour maps of the gas phase volume fraction, vapor mass fraction, pressure field, and gas temperature fields generated by the various methods are depicted in Figures 12, 13, 14, and 15 respectively. As can be seen, the overall structure of the various fields are similar even though there exist some variations in the details. The volume fraction fields (Figure 12) reflect the droplet velocity fields displayed in Figure 11, with the droplet volume fraction decreasing as droplets move in the domain. As expected, the vapor mass fraction (Figure 13) in the gas phase maximizes at exit from the domain with the full

multiphase results showing less evaporation in the region around the centerline of the domain. Pressure and temperature field maps presented in Figures 14 and 15 show similar profiles with slight variation in levels. This is further revealed in the comparison of profiles presented in Figure 16. In this figure, u-velocity, gas temperature, pressure, and vapor mass fraction profiles across the domain at $x=0.5$ generated using the various algorithms are compared. The gas u-velocity profiles (Figure 16(a)) obtained by the various methods are nearly coincident. The temperature profiles however (Figure 16(b)), show a slight difference in the region around the centerline of the domain, with profiles predicted by MUSIG and H-MUSIG being almost coincident. Pressure profiles presented in figure 16(c) show similar variations with values obtained with the full multiphase method being slightly higher. Moreover, profiles in Figure 16(d) show that H-MUSIG results are closer to the full multiphase results with the differences between the various profiles being in the region around the centerline and the largest evaporation rate being predicted by the full multiphase method.

CROSS-STREAM INJECTION INTO A SUPERSONIC STREAM IN A RECTANGULAR DOMAIN

The physical domain depicted in Fig. 4(b) is subdivided into 130×70 non-uniform control volumes. The length L of the domain is 1.1 m. The fuel is injected through 12 uniform control volumes (each of width $.001/12$ m) from two nozzles located on the lower and upper walls at 10 cm from the inlet. The Mach number and temperature of the air at inlet to the domain are taken to be 2 ($M_{\text{air,inlet}}=2$) and 700 K, respectively. The mixture of air and droplets are injected into the domain at a temperature of 350 K with the volume fraction of Kerosene in the injected air-fuel mixture being 0.01. The velocity of the injected mixture is 150 m/s and the angle of injection is 60° . With this velocity and volume fraction a total of 2.34 Kg/s/m of fuel are injected into the domain.

Full multiphase results are generated using 5 droplet phases of sizes of $60\ \mu\text{m}$, $80\ \mu\text{m}$, $100\ \mu\text{m}$, $120\ \mu\text{m}$, and $140\ \mu\text{m}$ with their inlet volume fractions being 0.0025, 0.0045, 0.006, 0.0045, and 0.0025, respectively. For the MUSIG model, the droplet phase is divided into 10 groups using the equal diameter discretization with the diameter of the smallest droplet set to $55\ \mu\text{m}$

and the increment to 10 μm with population fractions of 0.05, 0.075, 0.1, 0.125, 0.15, 0.15, 0.125, 0.1, 0.075, and 0.05, respectively. For the H-MUSIG model, two droplet phases are considered, each divided into five group sizes discretized using the equal diameter discretization. The diameters and population fractions of the various groups are similar to those used with MUSIG. The percentages of the injected fuel that has evaporated into the gas field as predicted by the various methods are found to be 10.64%, 13.25%, and 13.41% for the full multiphase method, the H-MUSIG model, and the MUSIG model respectively.

Comparison of results obtained using the various techniques are presented in Figures 17 through 22. Figure 17 displays the velocity fields for some of the droplet phases. Figure 17(a)-17(c) depicts the velocity vectors for droplet phases 1 (60 μm in diameter), 3 (100 μm in diameter), and 5 (140 μm in diameter) using the full multiphase approach. H-MUSIG droplet velocity vectors are presented in Figures 17(d) and 17(e), while Figure 17(f) shows the droplet vector field predicted using MUSIG. As in the streamwise injection case, the multiphase and the H-MUSIG results reveal a relatively larger droplet penetration with increasing droplet diameter. Further the path of the droplets predicted by MUSIG is between the trajectories of the smaller and larger droplet phases predicted by H-MUSIG (Compare Fig. 17(f) against Figures 17(d) and 17(e)). The same is true for H-MUSIG and the full multiphase results (compare Figure 17(d) against Figures 17(a) and 17(b); and Figure 17(e) against Figures 17(b) and 17(c)).

Comparisons in the form of contour maps of the gas phase volume fraction, vapor mass fraction, pressure field, and gas temperature fields generated by the various methods are depicted in Figures 18, 19, 20, and 21 respectively. The volume fraction fields (Figure 18) reflect the droplet velocity fields displayed in Figure 17, with the droplet volume fraction decreasing as droplets move in the domain. As expected, the vapor mass fraction (Figure 19) in the gas phase maximizes at exit from the domain. With the injection velocity used, droplets are not capable to penetrate into the central core of the domain. Pressure and temperature field maps presented in Figures 20 and 21 show similar profiles with slight variation in levels. Interaction of both injected streams via pressure is obvious.

In Figure 22, the u-velocity, gas temperature, pressure, and vapor mass fraction profiles across the domain at $x=0.6$ (i.e. at 0.5 m from the nozzles) generated using the various algorithms are compared. As in the previous cases, the gas u-velocity (Figure 22(a)) component and gas temperature (Figure 22(b)) profiles are nearly coincident. Moreover, pressure values (Figure 22(c)) are closer than in the previous cases with MUSIG and H-MUSIG profiles being on top of each others. Furthermore, vapor mass fraction profiles displayed in Figure 22(d) indicate that H-MUSIG results are closer to the full multiphase results with maximum differences between the various profiles occurring in the region close to the lower and upper walls.

STREAMWISE INJECTION INTO A SUPERSONIC STREAM IN A CYLINDRICAL DOMAIN

The physical domain depicted in Figure 4(c) representing the front view of the upper half of a cylindrical duct of length 1 m, is subdivided into 120x60 non-uniform control volumes. The fuel is injected through 12 uniform control volumes (each of width .001/12 m) from a nozzle located at the center of the domain, as shown in Figure 4(c). By neglecting body forces, the problem can be solved as an axi-symmetric two-dimensional one. The Mach number and temperature of the air at inlet to the domain are taken to be 2 ($M_{\text{air,inlet}}=2$) and 700 K, respectively. The mixture of air and droplets are injected into the domain at a temperature of 350 K with the volume fraction of Kerosene in the injected air-fuel mixture being 0.5. The velocity of the injected mixture is 150 m/s and the angle of injection varies between 0° and 60° , measured from the centerline of the nozzle. With this velocity and volume fraction a total of $2.01349\text{e-}2$ Kg/s/rad of fuel are injected into the domain.

Full multiphase results are generated using 5 droplet phases of sizes of $60\text{ }\mu\text{m}$, $80\text{ }\mu\text{m}$, $100\text{ }\mu\text{m}$, $120\text{ }\mu\text{m}$, and $140\text{ }\mu\text{m}$ with their inlet volume fractions being 0.0625, 0.1125, 0.15, 0.1125, 0.0625, respectively. For the MUSIG model, the droplet phase is divided into 10 groups using the equal diameter discretization with the diameter of the smallest droplet set to $55\text{ }\mu\text{m}$ and the increment to $10\text{ }\mu\text{m}$ with population fractions of 0.05, 0.075, 0.1, 0.125, 0.15, 0.15, 0.125, 0.1, 0.075, and 0.05, respectively. For the H-MUSIG model, two variations are

considered. In the first, two droplet phases are considered, each divided into five group sizes discretized using the equal diameter discretization. In the second, five droplet phases are considered, each divided into two group sizes using the equal diameter discretization. The diameters and population fractions of the various groups are similar to those used with MUSIG. The percentages of the injected fuel that has evaporated into the gas field as predicted by the various methods are found to be 9.38%, 8.66%, 10.2%, and 10.1% for the full multiphase method, the H-MUSIG model with five droplet phases, the H-MUSIG model with two droplet phases, and the MUSIG model respectively.

Comparison of results obtained using the various techniques are presented in Figures 23 through 28. Figure 23 displays the velocity fields for some of the droplet phases. Figure 22(a)-22(c) depicts the velocity vectors for droplet phases 1 (60 μm in diameter), 3 (100 μm in diameter), and 5 (140 μm in diameter) using the full multiphase approach. Figures 22(d)-(h) are for droplet velocity vectors predicted by H-MUSIG with Figures 22(d)-22(f) displaying veclocity vectors for the first, third, and fifth phases for the droplet phases case and Figures 22(g) and 22(h) being for the two droplet phases case. Moreover, Figure 22(i) shows the droplet vector field predicted using MUSIG. As for the previous cases, larger droplets show larger spreading due to their higher inertia.

Comparisons in the form of contour maps of the gas phase volume fraction, vapor mass fraction, pressure field, and gas temperature fields generated by the various methods are depicted in Figures 24, 25, 26, and 27 respectively. The general trend in variation resembles the previous cases, i.e. the volume fraction of the particles decreases in the stream-wise direction (Figure 24), and the mass fraction of the fuel vapor in the gas phase (Figure 25) increases in the streamwise direction as more kerosene evaporates. Pressure and temperature field maps presented in Figures 26 and 27 show similar profiles. In Figure 28, the u-velocity, gas temperature, pressure, and vapor mass fraction profiles across the domain at $x=0.5$ generated using the various algorithms are compared. As shown, the gas u-velocity (Figure 28(a)) component, gas temperature (Figure 28(b)), and pressure (Figure 28(c)) profiles are nearly coincident. Significant differences are notices in vapor mass fraction profiles (Figure

28(d)) and the increase in the number of phases in H-MUSIG has improved the profile away from the center where it is nearly coincident with the full multi-phase profile. However in the core region the 5 phases H-MUSIG solution predicts lower values than MUSIG and the two-phase H-MUSIG, which are closer to the full multi-phase values there.

CLOSING REMARKS

Three numerical methods following a full multiphase approach, (ii) a MUlti-Size Group (MUSIG) approach, and (iii) a Heterogeneous MUSIG (H-MUSIG) approach for the prediction of mixing and evaporation of liquid fuel injected into a stream of air flowing at any speed were developed. The numerical procedures were formulated, following a Eulerian approach, within a pressure-based fully conservative Finite Volume method. The $k-\epsilon$ two-equation model was used to account for the droplet and gas turbulence with modifications to account for compressibility at high speeds. The relative performance of the three approaches was assessed by solving for mixing and evaporation in three configurations involving droplets sprayed in the stream-wise and cross-stream directions in subsonic and supersonic streams flowing in rectangular and cylindrical domains.

Results, displayed in the form of droplet velocity vectors, contour plots, and axial profiles indicate that solutions obtained by the various techniques exhibit similar behavior. Differences in values are relatively small with the largest being associated with droplet volume fractions and vapor mass fraction in the gas phase. This is attributed to the fact that with MUSIG and H-MUSIG no droplet diameter equation is solved and the diameter of the various droplet phases are held constant, as opposed to the full multiphase approach. Results generated using MUSIG and H-MUSIG could be improved through better representation of evaporation in the population balance equations. This will form the subject of future developments.

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INVENTIONS

I certify that there were no subject inventions to declare during the performance of this grant

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FIGURE CAPTIONS

Figure 1 Schematic of the full multiphase approach.

Figure 2 Schematic of the MUSIG approach.

Figure 3 Schematic of the H-MUSIG approach.

Figure 4 Physical domain for (a) streamwise injection in a rectangular duct, (b) cross-stream injection in a rectangular duct, and (c) streamwise injection in a cylindrical duct; (d) an illustrative grid.

Figure 5 Velocity fields predicted by the full multiphase (a,b,c, in increasing droplet size), the HMUSIG (d, e, in increasing Sauter diameter) and the MUSIG (f) methods for streamwise injection in a subsonic flow field ($M_{in}=0.2$) in a rectangular domain.

Figure 6 Air volume fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a subsonic flow field ($M_{in}=0.2$) in a rectangular domain.

Figure 7 Vapor Mass fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a subsonic flow field ($M_{in}=0.2$) in a rectangular domain.

Figure 8 Pressure fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a subsonic flow field ($M_{in}=0.2$) in a rectangular domain.

Figure 9 Gas temperature fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a subsonic flow field ($M_{in}=0.2$) in a rectangular domain.

Figure 10 Comparison of (a) u-velocity, (b) temperature, (c) pressure, and (d) vapor mass fraction profiles across the domain at $x=0.5m$ generated using the full multi-phase, MUSIG, and H-MUSIG methods ($M_{in}=0.2$, Streamwise injection in a rectangular domain).

Figure 11 Velocity fields predicted by the full multiphase (a,b,c, in increasing droplet size), the HMUSIG (d, e, in increasing Sauter diameter) and the MUSIG (f) methods for streamwise injection in a Supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 12 Air volume fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 13 Vapor mass fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 14 Pressure fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 15 Gas temperature fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 16 Comparison of (a) u-velocity, (b) temperature, (c) pressure, and (d) vapor mass fraction profiles across the domain at $x=0.5m$ generated using the full multi-phase, MUSIG, and H-MUSIG methods ($M_{in}=2$, Streamwise injection in a rectangular domain).

Figure 17 Velocity fields predicted by the full multiphase (a,b,c, in increasing droplet size), the HMUSIG (d, e, in increasing Sauter diameter) and the MUSIG (f) methods for Cross-stream injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 18 Air volume fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for cross-stream injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 19 Vapor mass fraction fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for cross-stream injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 20 Pressure fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for cross-stream injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 21 Gas temperature fields predicted by the full multiphase (a), the HMUSIG (b), and the MUSIG (c) methods for cross-stream injection in a supersonic flow field ($M_{in}=2$) in a rectangular domain.

Figure 22 Comparison of (a) u-velocity, (b) temperature, (c) pressure, and (d) gas turbulent viscosity profiles across the domain at $x=0.5m$ generated using the full multi-phase, MUSIG, and H-MUSIG methods ($M_{in}=2$, cross-stream injection in a rectangular domain).

Figure 23 Velocity fields predicted by the full multiphase (a,b,c, in increasing droplet size), the HMUSIG with 5 droplet phases (2 groups per phase) (d, e,f, in increasing Sauter diameter), the HMUSIG with 2 droplet phases (5 groups per phase) (g, h, in increasing Sauter diameter), and the MUSIG (i) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a cylindrical domain.

Figure 24 Volume fraction fields predicted by the full multiphase (a), the HMUSIG with five droplet phases (2 groups per phase)(b), the HMUSIG with tow droplet phases (5 groups per phase)(c), and the MUSIG (d) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a cylindrical domain.

Figure 25 Vapor mass fraction fields predicted by the full multiphase (a), the HMUSIG with five droplet phases (2 groups per phase)(b), the HMUSIG with tow droplet phases (5 groups per phase)(c), and the MUSIG (d) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a cylindrical domain.

Figure 26 Pressure fields predicted by the full multiphase (a), the HMUSIG with five droplet phases (2 groups per phase)(b), the HMUSIG with tow droplet phases (5 groups per phase)(c), and the MUSIG (d) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a cylindrical domain.

Figure 27 Gas temperature fields predicted by the full multiphase (a), the HMUSIG with five droplet phases (2 groups per phase)(b), the HMUSIG with tow droplet phases (5 groups per phase)(c), and the MUSIG (d) methods for streamwise injection in a supersonic flow field ($M_{in}=2$) in a cylindrical domain.

Figure 28 Comparison of (a) u-velocity, (b) temperature, (c) pressure, and (d) vapor mass fraction profiles across the domain at $x=0.5m$ generated using the full multi-phase, MUSIG, and H-MUSIG methods ($M_{in}=2$, Streamwise injection in an Axi-Symmetric domain).