Simulation of evaporating isopropyl alcohol droplets injected into a turbulent flow

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Nomenclature

\[ B_M \] - mass transfer number; \[ B_T \] - thermal transfer number; 
\[ C_d \] - drag coefficient; \[ C_p \] - specific heat, J/kgK; 
\[ D_m \] - binary mass diffusivity coefficient; 
\[ h \] - enthalpy, J/kg; \[ J \] - mass flux, kg/m²s; 
\[ L_v \] - latent heat of vaporization, J/kg; 
\[ m_D \] - binary mass diffusivity coefficient; 
\[ m \] - mass flow rate, kg/s; 
\[ Sc \] - Schmidt number; 
\[ T_sc \] - Schmidt turbulent number; 
\[ Pr \] - Prandtl number; 
\[ T_pr \] - Prandtl turbulent number; 
\[ Re \] - Reynolds number; 
\[ S_m \] - mass source term; \[ S_e \] - energy dissipation source term; 
\[ g_T \] - gas temperature, K; \[ ST \] - droplet temperature surface, K; 
\[ U_g \] - droplets velocity, m/s; \[ U_s \] - gas velocity, m/s; 
\[ Y \] - mass fraction.

Greek symbols.

\[ \varepsilon \] - turbulent energy dissipation rate; \[ \phi \] - heat transfer rate; 
\[ \lambda \] - thermal conductivity, W/mK; \[ \nu \] - cinematic viscosity, m²/s; 
\[ \mu \] - dynamic viscosity, kg/ms; \[ \mu_t \] - turbulent dynamic viscosity; 
\[ \rho_L \] - droplet density; \[ \rho_g \] - gas density.

Subscripts.

\( d \) - droplet, \( F \) - fuel, \( g \) - gas, \( L \) - liquid, \( s \) - surface.

1. Introduction

Spray vaporization and combustion studies are of primary importance in the prediction and improvement of systems utilizing spray injection, in liquid fuelled combustion systems such as industrial boilers, gas turbines, direct ignition diesel engines, rocket and air-breathing engine applications. In these systems the vaporization is the dominant process, the fuel is injected into the combustion chamber. The spray is made of fine fuel droplets of different sizes. The fuel vapour mixes with the oxidizer gas to form the reactive mixture is ignited, which mixes to produce the spray combustion [1]. Usually the injection of the spray is in a turbulent flow, this accelerating the molecular diffusion of heat and species, the dominant factor for improved combustion efficiency and reducing the formation of pollutants such as unburned carbon monoxide and NOx. Many excellent reviews already exist on the various phenomena related to droplet motion and vaporization. The work on droplet motion is reviewed by Clift and Gauvin [2], Clift and al [3], Leal [4], The spray modeling work is reviewed by Williams [5], and Faeth [6], and the droplet vaporization models by Law [7], Sirignano [8], and Aggarwal and al [9]. The basic droplet vaporization model for an isolated single component droplet in a stagnant environment was formulated by Godsave [10], Spalding [11].

The aim of the present paper is to extend our model to turbulent jet applications, and to account for the two-way coupling between the fluid turbulent and the droplet heat transfers.

2. Assumptions and mathematical model

The following assumptions are considered in the present model:
- the droplet is assumed to be spherical;
- the spray is assumed to be dilute, under this assumption droplet collisions are ignored and the effect of adjacent droplets on droplet transport rates is neglected;
- the pressure is assumed to be constant and equal to the local mean ambient;
- equilibrium conditions at the droplet/gas interface are assumed;
- uniform physical properties of the surrounding fluid;
- the gas phase Lewis number is assumed to be unity in the droplet mode;
- radiation between the droplets and their surroundings is neglected;
- temperature inside the droplet is uniform.

3. Droplets vaporization

Under steady state vaporization, solutions of the species conservation and energy equations are obtained by analyzing the interface flux conditions between the liquid and gas phases (Fig. 1).

3.1. Mass conservation

With the assumption of quasisteady vapourisation, the mass flow rate is constant, independent of radius.

\[ \text{div}(\rho \vec{v}) = \frac{1}{r^2} \frac{d}{dr} (r^2 \rho v_r) = 0 \] (1)

\[ 4 \pi r^2 \rho v_r = \dot{m} = \text{constant} \] (2)

where \( \dot{m} \) is the mass transfer rate from the droplet to the air; \( v_r \) is the radial velocity.
3.2. Mass conservation of the fuel vapor

The presence of the oxidant around the droplet during the evaporation process is not necessary. Therefore, only the fuel vapor is considered

\[
\frac{d}{dr} \left( 4 \pi \rho_s r^2 v_s Y_f \right) = \frac{d}{dr} \left( 4 \pi \rho_s D_m r^2 \frac{dY_f}{dr} \right)
\]

or

\[
\dot{m} Y_f - 4 \pi r^2 \rho_s D_m \frac{dY_f}{dr} = \dot{m} = \text{const}
\]

with \( Y_f \) is the fuel mass fraction; \( D_m \) is the binary mass diffusivity.

By integration of equation (3) using the boundary conditions

\[
r = r_s, \; Y_f = Y_{f_s}
\]

\[
r = \infty, \; Y_f = 0
\]

where we obtain the profile of the fuel mass fraction and mass flow of spray

\[
Y_f = 1 - \exp \left( -\frac{\dot{m}}{4\pi\rho_s D_m r} \right)
\]

\[
\dot{m} = 4 \pi \rho_s D_m r \ln(1 + B_u)
\]

where

\[
B_u = \frac{Y_{f_s} - Y_f}{1 - Y_{f_s}}
\]

3.3. Energy conservation

\[
\text{div} \left( \rho \vec{v} \right) = \text{div} \left( \Phi \sum_i h \vec{j}_i \right)
\]

where

\[
\Phi = -\lambda \text{grad} \left( T \right) \quad \text{(Fourier’s law)}
\]

\[
\vec{j}_i = -\rho D_i \text{grad} \left( Y_i \right) \quad \text{(Fick’s Law)}
\]

Because the transfer of heat from the environment to the droplet is only by conduction, the equation of energy conservation is given by

\[
\frac{d}{dr} \left( 4 \pi \rho_s r^2 v_s C_p T \right) = \frac{d}{dr} \left( 4 \pi r^2 \lambda \frac{dT}{dr} \right)
\]

By integration of Eq. (11) using the boundary conditions:

\[
r = r_s, \; T = T_s
\]

\[
r = \infty, \; T = T_{\infty}
\]

where we obtain the temperature profile in the gas phase and the vaporized mass flow

\[
T = T_s - \frac{L_v}{C_p} \left( T_{\infty} - T_s + \frac{L_v}{C_p} \exp \left( -\frac{\dot{m}}{4\pi\rho_s D_m r} \right) \right)
\]

\[
\dot{m} = 4 \pi \rho_s D_m r \ln(1 + B_t)
\]

where

\[
B_t = \frac{C_p(T_{\infty} - T_s)}{L_v}
\]

On taking into account the stationary system

\[
B = B_{M_0} = B_t
\]

The expression for a vaporization process in a quiescent surrounding air

\[
\frac{dD_M^2}{dt} = -8\frac{\rho_s}{\rho_l} D_m \ln(1 + B)
\]

In the present of significant convection, the change of droplet diameter is represented as follows, Ranz and Marshall [12]

\[
\frac{dD_M^2}{dt} = -8\frac{\rho_s}{\rho_l} D_m \ln \left( 1 + B \left( 1 + 0.3Re^{0.74}Pr^{13} \right) \right)
\]

3.4. Droplet dynamics

The droplet dynamics are simulated using a Lagrangian point-particle model and the equation governing the droplet motions can be written [13]

\[
\frac{dU_j}{dt} = -3 \frac{\rho_s C_d}{4 \rho_s D} \left( U_j - U_i \right) \left( U_j - U_i \right) + \frac{(\rho_d - \rho_s)}{\rho_d} \left( \rho_d - \rho_s \right)
\]

where \( C_d \) is the drag coefficient that depends on the Reynolds number for a spherical configuration of the droplet

\[
\begin{align*}
C_d &= \frac{24}{Re}, \quad &Re < 1 \\
C_d &= \frac{24}{Re} \left( 1 + 0.15Re^{0.87} \right), \quad &Re \leq 1000 \\
C_d &= 0.438, \quad &Re > 1000
\end{align*}
\]
\[ Re = \frac{|U_a - U_g| D}{v_r}. \]  

4. Gas phase

The vapor produced by the droplets is a mass source for the fluid, moreover the vaporization process generates modification in the momentum and energy balances both phases. Fluid phase equations then contain many extra source terms. Assuming that the vapor production does not modify the liquid phase density, the governing equations read as follows Berlemont et al [14]

4.1. Continuity equation

\[ \frac{\partial}{\partial x_i} (\rho U_i) = \tilde{S}_m \]  

where \( \tilde{S}_m \) is the mass source term.

4.2. Momentum equation

\[ \frac{\partial}{\partial x_j} (\rho U_j) = -\frac{\partial}{\partial x_j} \left[ P + \frac{2}{3} \rho k \right] + \frac{\partial}{\partial x_j} \left[ 2 \mu + \mu_t \right] \frac{\partial U_j}{\partial x_j} + \frac{\partial}{\partial x_j} (\mu + \mu_t) \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \tilde{S}_m \]  

where \( \tilde{S}_m \) is the momentum source term.

4.3. Energy equation

\[ \frac{\partial}{\partial x_j} (\rho U_j T) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr} \right) \frac{\partial T}{\partial x_j} + \tilde{S}_\mu + \tilde{S}_m \]  

where \( \tilde{T} \) is the mean temperature; \( \tilde{S}_\mu \) is the enthalpy source term.

4.4. Mean vapor mass fraction

\[ \frac{\partial}{\partial x_j} (\rho U_j Y) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc} \right) \frac{\partial Y}{\partial x_j} \]  

where \( Sc \) and \( Sc_r \) are the Schmidt and Schmidt turbulent number, respectively.

4.5. Turbulent equations

Fluid turbulence is still described using a \((k-\epsilon)\), but the modification of the continuity equation leads to extra terms in the \(k\)-equation, \(\epsilon\)-equation and for energy and vapor mass fraction equations.

4.5.1. The kinetic energy equation

\[ \frac{\partial}{\partial x_j} (\rho U_j k) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{\sigma_k} \right) \frac{\partial k}{\partial x_j} + \tilde{\xi}_k \]  

where

\[ \tilde{\xi}_k = G - C_D \rho \epsilon + \tilde{S}_k \]  

\[ G = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \]  

where \( G \) is the turbulent energy production term; \( \tilde{S}_k \) is the extra source term.

4.5.2. Energy dissipation rate equation

\[ \frac{\partial}{\partial x_j} (\rho U_j \tilde{\epsilon}^2) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \tilde{\epsilon}^2}{\partial x_j} + \tilde{\xi}_\epsilon \]  

where

\[ \tilde{\xi}_\epsilon = C_{\epsilon 1} \tilde{\epsilon} G - C_{\epsilon 2} \rho \frac{\tilde{\epsilon}^2}{k} + \tilde{S}_\epsilon \]  

\( \tilde{S}_\epsilon \) is the energy dissipation source term.

4.5.3. Scalar fluctuation transport equation

\[ \frac{\partial}{\partial x_j} (\rho U_j \tilde{Y}) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc} \right) \frac{\partial \tilde{Y}}{\partial x_j} \]  

with

\[ \tilde{\xi}_\theta = C_{\theta 1} H \frac{\partial \tilde{T}}{\partial x_j} \]  

\( C_D = 1, \sigma_k = 1, \sigma_\epsilon = 1.3, \sigma_\theta = 1.92 \),

\( C_{\epsilon 1} = 1.44, C_{\epsilon 2} = 1.92, C_{\theta 1} = 2.8, C_{\theta 2} = 1.92 \).

5. Computational details

Fig. 2 shows a schematic of the computational domain used for the model coaxial combustor investigated by Sommerfeld and Qiu [15]. The chamber consists of an annular section discharging hot air into a cylindrical test section. The central section consists of a nozzle through which isopropyl alcohol at 313 K is sprayed into the test section. Hot air at constant temperature of 373 K enters the annulus. The boiling temperature of isopropyl alcohol at atmospheric pressures is 355 K and thus the evaporation is dominated by mass transfer effects. The air and liquid mass flow rates are 28.3 and 0.44 g/s, respectively. The over all mass loading is small resulting in a dilute spray. The outer radius of the annulus \( r = 32 \) mm. The mean axial inlet velocity in the annular section is 18 m/s.

The numerical simulation is performed by using the industry code "FLUENT" which uses a numerical method to finite volume coupled with a multigrid resolution scheme. The flow governing equations are solved by using a performed SIMPLE algorithm and using the stan-
standard $k-\varepsilon$ model of turbulence.

Fig. 3 shows the computational grid used. The configuration of the jet is considered to be axisymmetric. The definitions of the geometry and mesh generation were performed by using the Gambit mesh with a quadrilateral mesh of shape. The area is modelled for dimensions of radius 100 mm and 350 mm in length that corresponds to a half cylinder.

The mesh consists of 100 nodes in the radial direction and 80 nodes in the axial direction. The stitches are tightened in the area near the injector.

6. Results and discussion

6.1. Flow without injection

First, the single-phase air flow through the model combustion chamber is simulated (without injecting any liquid droplets). The radial variations of the mean and RMS axial velocity field at different axial locations are compared with the experimental data.

The results of Figs. 4 and 5 show the evolution of the mean axial velocity as a function of the distance to the plane of the injector at distances 25 and 50 mm. In these figures the radial mean velocity is negative near the jet axis; this is due to internal circulation of the flow at the entrance of the jet.

![Axial mean velocity profile at 25 mm](image)

![Axial mean velocity profile at 50 mm](image)

The annular flow is also characterized by a peak velocity of 18 m/s between 20 and 30 mm in Fig. 4.

The results of Figs. 6 and 7 show the evolution of the mean radial velocity as a function of radial distance to the plane of the injector at distances 25 and 50 mm. In these figures the radial mean velocity is negative near the jet axis; this is due to internal circulation of the flow at the entrance of the jet.

![Radial mean velocity profile at 25 mm](image)

Figs. 8-10 and 11 show the results of the RMS axial and radial velocity as a function of the distance to the
plane of the injector at distances 25 and 50. We observe in these figures that these results are in good agreement with experimental results with a small overestimate; this overestimation is expected because the axial and radial fluctuations are almost identical in the prediction while a strong anisotropy is observed in the experience and this anisotropy is difficult to reproduce by simulation.

6.2. Flow with droplets injection

The study of the flow without evaporation gave a good agreement with the experimental configuration of Sommerfeld and Qiu [15]. We will resume this configuration by injecting a spray of isopropyl alcohol in the center of the flow to fully test our model and compare our results with the measured results. The flow rate of the liquid injected is 0.443 g/s, and the outlet temperature of injector is 313 K. The ambient temperature is 373 K. The mean axial velocity of the gas flow is 18 m/s. The initial droplet diameter in the inlet is 20 to 50 μm.

The results of axial mean velocities of the droplets are shown in Figs. 12 and 13 for two different distances to the plane of the injector. These results are in a good agreement with experimental results with a small overestimate.

The results of radial mean velocities of the droplets are shown in Figs. 14 and 15. These figures show the distributions of the mean diameter as a function of the distance to the plane of the injector at distances of 25 and 50 mm. We observed in these figures that the distribution is at a pace backward, and although this profile due to initial injection.
The results have a good overall agreement with experimental results measured at the entrance plane of the tube with a small overestimation of the plans from the tube.

Fig. 12 Droplets velocity at 25 mm

Fig. 13 Droplets velocity at 50 mm

Fig. 14 Droplets diameter at 25 mm

Fig. 15 Droplets diameter at 50 mm

Fig. 16 Mass fraction contours

Fig. 17 Droplets size distribution

7. Conclusion

The study we have presented is intended to properly compare our results with numerical experiments. Simulating the flow without injection gives a better approach for axial and radial mean velocity. The RMS axial and radial velocities are in good agreement with experimental results with a small overestimate, this overestimation is expected because the axial and radial fluctuations are almost identical in the model of simulation while a strong anisotropy is observed in the experience and this anisotropy is difficult to reproduce by simulation. We also note that apart from the axial zone that is to say from the vicinity of the injection and inside the jet. This is due to holding of the circulation droplets near the nozzle where they evaporate.
40 mm, the turbulence is very low due to poor circulation. We also note that the droplets follow the flow and differ very little from the gas jet.

The results of the axial mean velocities of the droplets are in good agreement with experimental results with a small overestimate.

References


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