

NUMERICAL MODELLING OF TURBULENCE EFFECTS WITHIN AN EVAPORATING DROPLET IN ATOMIZING SPRAYS

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Abstract

A new approach to account for finite thermal conductivity and turbulence effects within atomizing liquid sprays is presented in this paper. The model is an extension of the T-blob and T-TAB atomization/spray model of Trinh and Chen (2005). This finite conductivity model is based on the two-temperature film theory, where the turbulence characteristics of the droplet are used to estimate the effective thermal diffusivity within the droplet phase. Both one-way and two-way coupled calculations were performed to investigate the performance of this model. The current evaporation model is incorporated into the T-blob atomization model of Trinh and Chen (2005) and implemented in an existing CFD Eulerian-Lagrangian two-way coupling numerical scheme. Validation studies were carried out by comparing with available evaporating atomization spray experimental data in terms of jet penetration, temperature field, and droplet SMD distribution within the spray. Validation results indicate the superiority of the finite-conductivity model in low speed parallel flow evaporating spray.

Nomenclature

A_d	Droplet surface area (m^2)	q_l	Heat transfer rate from droplet surface to droplet core
B_m	Gas phase mass transfer number	q_g	Heat transfer rate from gas phase to droplet surface
C_d	Discharge coefficient of injector nozzle (0.7)	r_d	Droplet radius (m)
C_p	Specific heat capacity of mixture (KJ/kg K)	Sh_g	Gas phase Sherwood number
C_μ	Turbulence constant	T_b	Fuel boiling temperature (K)
\bar{D}	Binary Diffusivity (m^2/s)	T_d	Bulk temperature of droplet (K)
K_c	Loss coefficient due to nozzle inlet geometry (0.45)	T_g	Ambient gas temperature (K)
K_ϵ	Proportionality constant (0.23)	T_s	Droplet surface temperature (K)
k_l	Turbulent kinetic energy of the liquid (m^2/s^2)	s	Area ratio at nozzle contraction (0.0 for this study)
L_v	Latent heat of the fuel at the surface temperature (KJ/kg)	α_{eff}	Effective thermal diffusivity (m^2/s)
m_d	Droplet mass (kg)	α_{lam}	Laminar thermal diffusivity (m^2/s)
Nu_g	Gas phase Nusselt number	α_{turb}	Turbulent thermal diffusivity (m^2/s)
Pr_t	Turbulent Prandtl number (0.9)	λ_l	Liquid thermal conductivity
P_{atm}	Atmospheric pressure (Pa)	λ_g	Gas thermal conductivity (KW/m K)
P_{gas}	Gas phase pressure (Pa)	ϵ_l	Turbulent dissipation rate (m^2/s^3)
		δ_e	Equivalent thickness of thermal boundary layer (m)

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, the combustion performance is highly dependent on effective liquid fuel atomization and its subsequent evaporation processes. In evaporating sprays, the multi-phase gas-liquid flows for most practical situations involve the vaporization of droplets in high temperature convective gas streams with turbulent environments. These situations involve a dispersed liquid phase species in the form of a large number of discrete droplets convecting and vaporizing in a continuous gas phase species. As the liquid enters the hot free stream through a high velocity injector, atomization processes break up the liquid into droplets. During this process, only a fraction of the liquid droplet near the liquid/gas interface heats up while the core region remains cold. The heat transfer through molecular conduction and convection inside the droplet proceeds until the end of its lifetime. The liquid injector flow may produce droplet parcels with internal turbulence; in addition, high relative velocity between gas and droplets also generates internal circulation (such as vortex motion). To account for these convective effects, complex multi-dimensional models involving isolated droplet are required [e.g., Abramzon and Sirignano (1989)]. However, the high computational costs associated with resolving the temperature profile within an individual droplet is prohibitive for multi-dimensional spray combustion simulations.

On the other hand, the classical constant droplet-temperature model (D^2 law) or infinite conductivity (perfect mixing within the liquid droplets) models are often used for spray combustion simulation. Droplet evaporation rates predicted by liquid-side infinite conductivity (I-C) models tend to over predict or under predict the evaporation mass flux, depending on the ambient temperature conditions. Bertoli and Migliaccio (1999) showed that the accuracy of CFD computations of heating, evaporation and combustion of diesel fuel sprays could be substantially increased if the assumption of infinitely high thermal conductivity of liquid is relaxed. Simplified modelling approaches have been proposed to account for finite conductivity (F-C) effects within the evaporating droplets based on approximated analytical temperature profiles within liquid droplet [e.g. Tong and Sirignano (1986), Sazhin et al. (2005)]. Within the simplified models, the two-temperature formulations, in which the finite-conductivity effect is modelled by the temperature difference between the droplet surface temperature and a droplet "core" temperature, have been proposed recently. In the model of Renksizbulut et al. (1992), the difference between the surface and core temperature was related to the heat flux at the droplet surface by a constant Nusselt number. Zeng and Lee (2002) developed a zero-dimensional model, in which, the difference between surface and core temperature was traced by an ordinary differential equation (ODE) to account for the non-uniform distribution of temperature inside the droplet. The ODE two-temperature model was also used by Miller et al. (1998) to account for non-equilibrium Langmuir-Knudsen evaporation modelling. Ra and Reitz (2003) used a thermal boundary layer within the droplet to account for the finite-conductivity effect. The thermal boundary layer thickness was calculated using the thermal diffusivity model of Abramzon and Sirignano (1989) to account for the droplet internal circulation.

In this paper, a new finite-conductivity model is developed based the two-temperature formulation. This finite-conductivity effect is phenomenologically modelled through a thermal boundary layer within the droplet. The thermal diffusivity is calculated based on the turbulent characteristics within the droplet. The current study is an extension of a recently developed atomization/spray model [Trinh and Chen (2005)], the T-blob/T-TAB model, to include spray evaporation effects. Due to the unique feature of T-blob/T-TAB, in which the turbulence characteristics is accounted for within the droplet phase, extension of this model to include finite conductivity effect in the evaporating droplet can be made naturally. The model development will be described in this paper. Validations for one-

way coupling one-dimensional and two-way coupling multi-dimensional evaporating sprays will be presented.

2. Theory and Numerical Approaches

The current vaporization model is developed for computational analysis based on the Eulerian-Lagrangian numerical approach. In this formulation, the spray/droplets dynamics is described in a Lagrangian coordinate such that numerical droplets are tracked within the Eulerian gas dynamics. Liquid phase is tracked from the injector plane, and the primary atomization, as well as the subsequent secondary break-up is modelled using the T-blob/T-TAB hybrid model of Trinh and Chen (2005). Both primary and secondary droplet break-up processes are modelled and the transition from primary to secondary break-up is modelled based on energy balance. In addition to the droplets position and velocity, liquid turbulence is accounted for, through the injector characteristics by the two-equation k - ε turbulence model formulation using the T-blob/T-TAB model. The inherent turbulence in the injected fuel spray affects the heat and mass transfer rates of the vaporization process. The effects of these changes in the rates have to be accounted for in the numerical models for spray evaporation. Detailed model description and validations can be found in Trinh and Chen (2005), and it is suffice to say that within each numerical droplet, turbulence characteristics such as fluctuating velocity level, length and time scales are supplied by the model.

To utilize the T-blob/T-TAB model liquid jet atomization, turbulence characteristics need to be specified as the inlet boundary conditions. Based on integral analysis of straight injector [Trinh and Chen (2005)], liquid turbulent kinetic energy and its dissipation rate at the injector nozzle exit are estimated from:

$$k_i^o = \frac{U^2}{8L/D_{\text{nozzle}}} \left[\frac{1}{C_d^2} - K_c - (1-s^2) \right] \quad (1)$$

$$\varepsilon_i^o = K_e \frac{U^3}{2L} \left[\frac{1}{C_d^2} - K_c - (1-s^2) \right], \quad (2)$$

where L is the length of the injector nozzle, D_{nozzle} is the nozzle diameter, and the jet injection velocity U . A set of ODEs' were derived to track the evolution of k_i and ε_i within the droplet according to the T-blob/T-TAB model. The values obtained from the evolution of k_i and ε_i are used in the heat transfer calculations of the evaporation model.

To relax the infinite-conductivity, thus perfect mixing, assumption within the liquid droplet, a "two-temperature model" is formulated. In the two-temperature model, the core (or bulk) temperature (T_d), is assumed well-mixed by convection/turbulence transport. In consistence with the "film theory", heat resistance exists at the near surface region, and the droplet surface temperature (T_s) differs from the droplet core temperature. The heat transfer coefficient across this thin film (or boundary layer) is then formulated through the turbulence characteristics supplied from the T-blob/T-TAB model, to account for the finite conductivity effect. In the Lagrangian coordinate, the heat-up of the droplet core is formulated as:

$$m_d C_p \frac{dT_d}{dt} = h_1 (T_s - T_d) A_d \quad (3)$$

where, h_1 is the liquid-side heat transfer coefficient and A_d is the droplet surface area. The heat transfer coefficient is determined from the thermal conductivity and a thermal boundary layer formulation [Sirignano (1999)] as:

$$h_1 = \frac{\lambda_l}{\delta_e}, \quad (4)$$

where λ_l is the liquid thermal conductivity. Using an unsteady equivalent boundary layer thickness, the film thickness, δ_e , is given by $\sqrt{\pi \alpha_{eff} t}$. The time scale t is estimated based on the mass transfer-limited integration time step Δt_{evap} (see details in section 3). The effective thermal diffusivity (α_{eff}), based on the turbulence characteristics within the droplet, is estimated from: $\alpha_{eff} = \alpha_{lam} + \alpha_{turb}$, in which the turbulent thermal diffusivity is calculated from the two-equation turbulence model diffusivity formulation:

$$\alpha_{turb} = \frac{C_\mu k_1^2}{Pr_t \varepsilon_1}, \quad (5)$$

here Pr_t is the turbulent Prandtl number and is set to be 0.9. The liquid droplet turbulence quantities k_1 and ε_1 are obtained from the T-blob/T-TAB atomization/spray model. In cases where gas phase diffusivities are much larger than liquid diffusivities, the droplet core heating will be rate controlling and the gas-side heat/mass transfer will respond in a quasi-steady manner. The surface temperature of the droplet is determined from a heat and mass transfer balance at the interface between the droplet and the surrounding gas assuming no heat accumulation at the droplet surface such that:

$$L_v \dot{m}_d = q_g - q_l \quad (6)$$

where L_v = latent heat of the fuel at the surface temperature, q_g = heat transfer rate from the environmental gas to the surface. In this paper, the classical Spalding evaporation model is used to model the gas-phase transport, thus the gas heat transfer rate was calculated as:

$$q_g = 2\pi D_p \lambda_g Nu_g (T_g - T_s) \frac{\ln(1+B)}{B} \quad (7)$$

q_l = heat transfer rate from the droplet interior to droplet surface

$$q_l = \frac{\lambda_l (T_s - T_d)}{\delta_e} A_s \quad (8)$$

and the evaporation rate at the surface is given as:

$$\dot{m}_d = \frac{dm_d}{dt} = 2\pi D_p (\rho_g \bar{D}) Sh_g \ln(1+B_m) \quad (9)$$

In the above equation, B_m is the Spalding mass transfer number, Sh_g is the Sherwood number, and \bar{D} is the binary diffusivity. The Sherwood and the Nusselt numbers were calculated using the classical correlations, given by:

$$Nu_g = 1 + 0.3 Re_p^{0.5} Pr^{0.333} \quad (10)$$

$$Sh_g = 1 + 0.3 Re_p^{0.5} Sc^{0.333} \quad (11)$$

The solution algorithm used in this study starts with an estimated surface temperature (T_s) at a new time step. The Clausius-Clayperon equation and the Raoult's law then are used to calculate the fuel vapour molar fraction followed by the calculation of the evaporation rate. An estimation of T_d is also required to simultaneously satisfy equations (3) and (6). More detailed iterative procedure can be found in Balasubramanyam (2006).

3. Results and Discussion

3.1 One-Way Evaporating Atomizing Spray

This case is an extension of the one-way T-blob/T-TAB testing case described in Trinh and Chen (2005). The Tridecane fuel was issued through a long injector tube at 300°K. The length of the injector nozzle (L) is 0.8 mm and the nozzle diameter (D_{nozzle}) is 0.3 mm. A jet injection velocity (U) of 102 m/s was used for one of the test cases. The environment is quiescent nitrogen at a

temperature of 600°K. The gas properties were calculated based on the reference state determined from the ‘1/3rd’ rule [Sirignano (1999)]. In this calculation, a ‘blob’ of numerical droplet was injected at the orifice plane with orifice diameter. The droplet then went through first and secondary break-up processes, thus its diameter decreased in time. The variation of the thermal boundary layer within the droplet also changed in time. A FORTRAN program was written for the one-way coupled evaporating atomizing spray in a quiescent gas. The purpose here is to investigate the concept of boundary layer film thickness within liquid droplets involving two temperatures. In the course of study, it was found that, due to the fact, in the secondary break-up regime (i.e. the T-TAB regime) the droplets were so small they were heated up rapidly. Thus the current model was only implemented within the T-blob (i.e., the primary break-up) model. As mentioned in section 2, the time scale in the thermal film thickness is evaluated based on the mass transfer-limit time step, and formulated as: $\Delta t_{\text{evap}} = \frac{\rho_l dV}{\mu_l Sh(4\pi r_d)}$ [Shang (1992)]. This time scale should be independent of the

integration time step used in numerical calculations. In figure 1, the sensitivity of integration time step on the calculation of the droplet thermal film thickness, normalized with droplet radius, is shown for several time step sizes. It can be seen that the results show good “time-step independency” in thermal boundary layer evolution within the droplet.

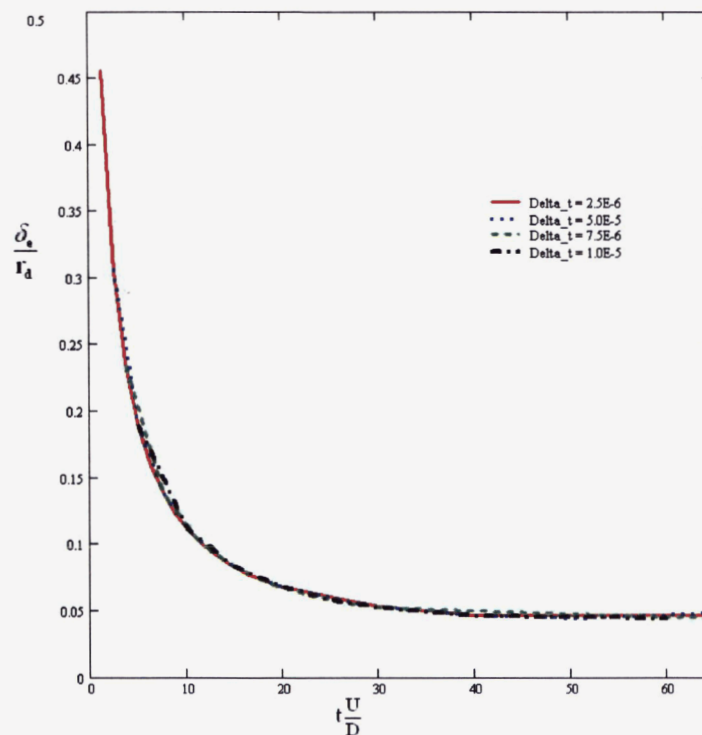


Figure 1. Variation of the normalized thermal boundary layer with time

The results also indicate that the normalized thermal boundary layer thickness is rather thick in the initial stage, decreases quickly to rather small value, and exhibits reasonable physical trend. It should be noticed that the current model gives thinner thermal boundary layer thickness when compared with the limiting thermal layer thickness based on internal vortex convection model. Utilizing the model of Abramzon and Sirignano (1989), Ra and Reitz (2003) suggested that the value of thermal layer thickness be limited to 1/2.257 of the droplet radius. It was also observed that, based on the current model, the turbulent diffusivity within the droplet was about two orders of magnitude higher than the laminar thermal diffusivity. The turbulent thermal diffusivity decreased in tandem with the decrease in the kinetic energy experienced by the drop. The variation of the drop surface temperature (T_s) and the bulk temperature of the drop (T_d) for the finite conductivity

(F-C) model in comparison with the bulk temperature calculated using the infinite conductivity (I-C) model is shown in figure 2.

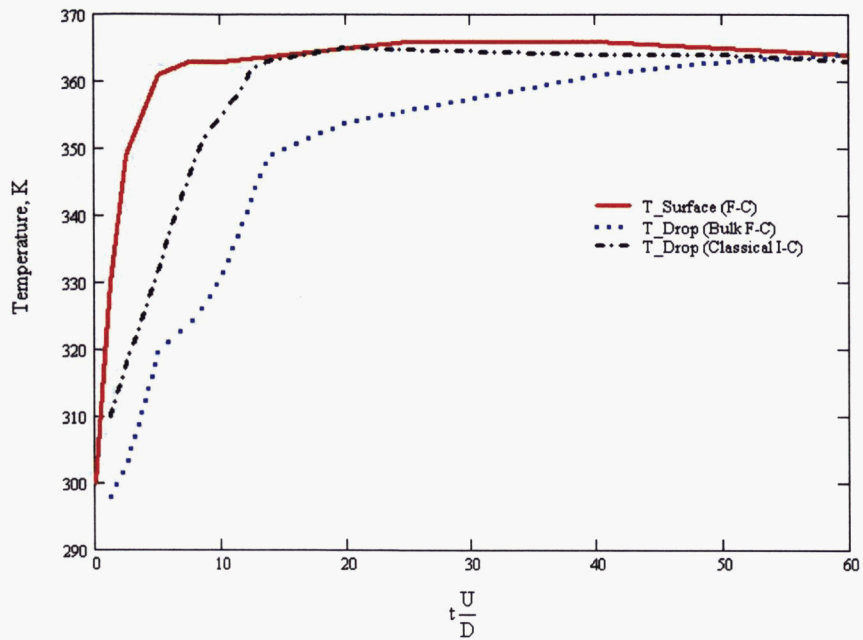


Figure 2. Droplet temperature history comparisons for the F-C and I-C models

The variation of the normalized parent drop radius with time for a one-way coupled test case, with iso-octane fuel evaporating in a quiescent environment is shown in figure 3. The rate of change in

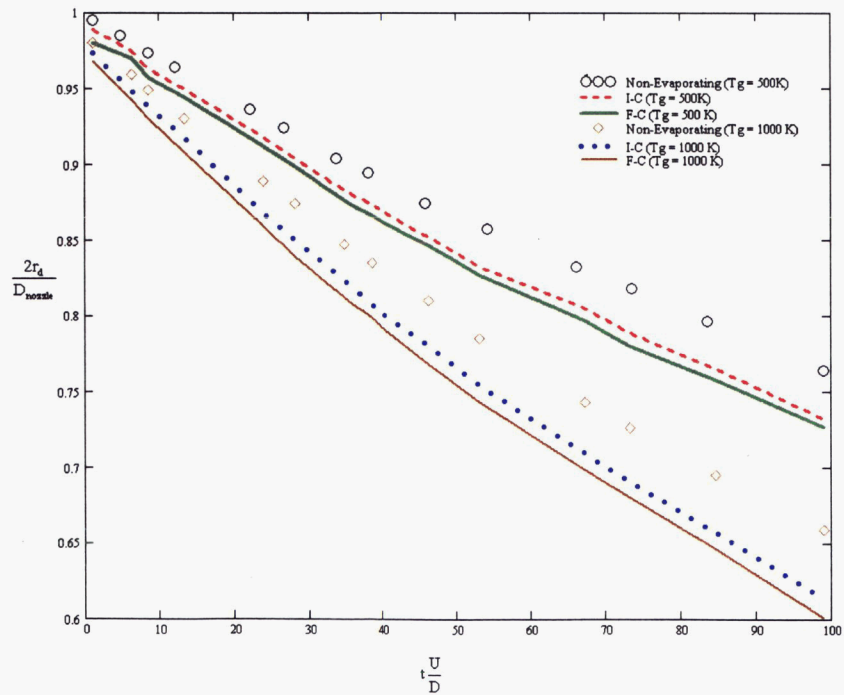


Figure 3. Comparative change in drop size for the F-C and I-C models

the radius, calculated based on the surface temperature is slightly higher than that calculated base on the bulk temperature of the droplet. The difference in rates increases with increase in ambient temperature.

The next step in the numerical development of the model was to validate its efficiency for applications in practical situations. To this effect, the model was then incorporated into the finite volume commercial CFD code ACE+ (2004). Validation of the code with test cases for which experimentally measured data is available for comparison was performed. Detailed numerical implementation (such as grids and time steps) can be found in Balasubramanyam (2006). Some of these results will be presented in this paper.

3.2 Two-Way Coupled Evaporating Spray Validation

To evaluate the current evaporation model, the 2-D axis-symmetric subsonic low-speed evaporating spray of Yakota et al. (1988) was tested first for a two-way coupling CFD calculation since a similar non-evaporating test case was used for the T-blob/T-TAB validation study [Trinh et al., 2005]. Liquid fuel (Tridecane, $C_{13}H_{28}$) is injected through a single-hole nozzle into a high pressure, high temperature ambient N_2 environment. The initial test conditions for the evaporating spray are summarized in Table 1.

Table 1. Test Conditions for the Measurement of Yakota et al. (1988)

Case	P_{inj}	P_{gas}	T_{amb}	M_{inj}	Gas Environment
Y - 1	30 Mpa	3 Mpa	900 K	0.00326 kg/s	N_2

The nozzle diameter was 0.16 mm. Equations (1) and (2), with the same values for nozzle parameters except for nozzle diameter and jet velocity, were used to estimate the initial liquid turbulence quantities. A computational domain of 20 mm in radius and 100 mm in length discretized by a 50 radial x 75 axial grid was used. The mesh spacing was non-uniform with refinement on the centreline and close to the injector. A constant time step of $2.5E-6$ sec. was used with an injection period of 4 μ sec. The properties of liquid fuel Tridecane were taken from the NIST/JANAF database. Estimating the penetration of a fuel jet into an air stream is an important global property for model validation and is presented first. In figure 4, the predicted tip penetration results using the current finite-conductivity (F-C) evaporation model coupled with the T-blob/T-TAB atomization model are compared with the measured data. For reference, predictions using classical Blob/TAB/infinite-conductivity (I-C) model, as well as using T-blob/T-TAB/infinite-conductivity model are also shown in the same figure. In figure 5, the corresponding droplet Sauter mean diameter (SMD) profiles along the jet axis are shown. It can be seen that the infinite-conductivity evaporation models tend to over predict the evaporation rate, thus gave shorter tip penetration. On the other hand, the finite-conductivity model slows down the evaporation process, and produce larger droplets and longer penetration. It should be noted that the coalescence model [Trinh and Chen (2005)] was used for all two-way coupling calculation cases. The coalescence model is responsible for the calculated overshoot phenomena observed in the initial period of injection for all simulated cases.

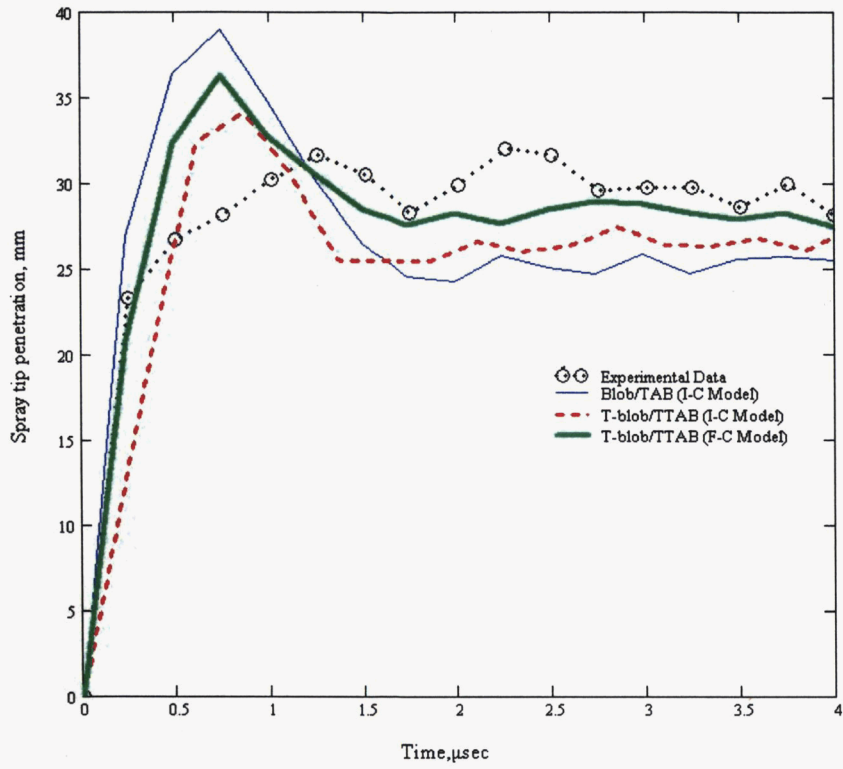


Figure 4. Spray tip penetration with time comparisons

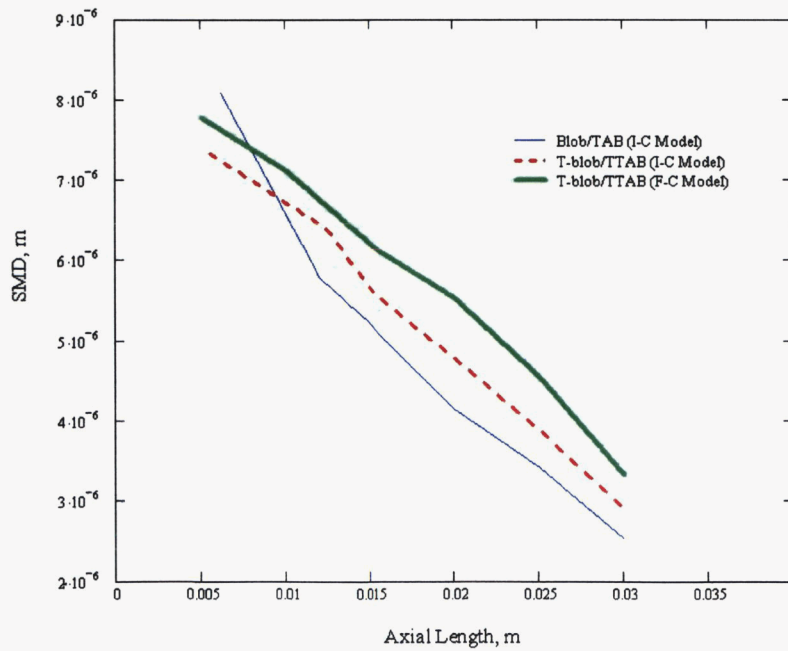


Figure 5. Sauter mean diameter (SMD) comparisons at centreline

The heat and mass transfer aspects of the evaporating jet are shown in figures 6 and 7 at time of 4 μ sec after injection. As can be observed, the models incorporating the turbulence effects in the primary and secondary atomization processes give more reasonable qualitative pictures when compared with the classical atomization model without liquid turbulence effect. Comparing figures 6.b and 6.c, the surface temperature contours predicted by the current finite-conductivity model show the effect of slowing down the rate of evaporation, based on the turbulence levels experienced by the individual droplets, rather than the constant drop temperature assumption of the classical infinite conductivity model.

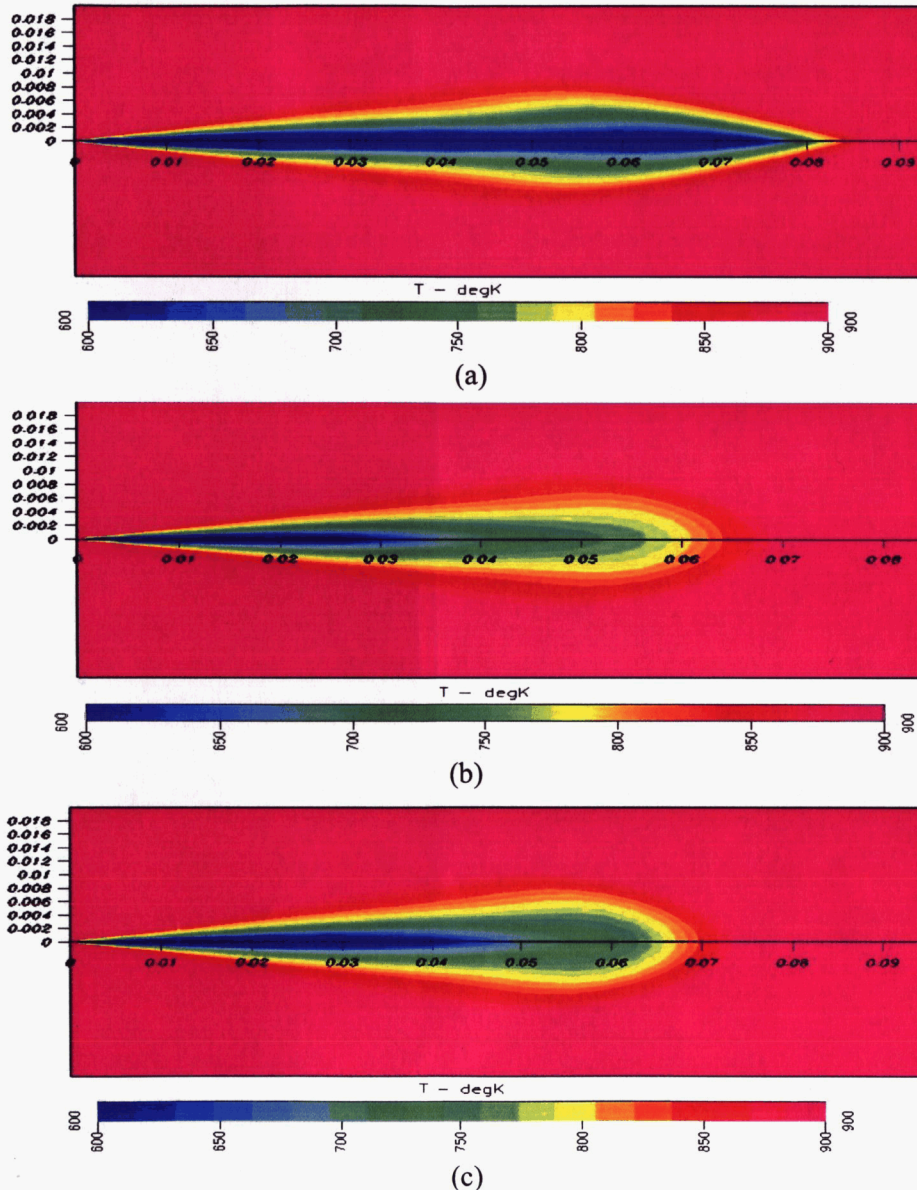


Figure 6. Temperature Contours at 4 μ sec; (a) I-C with Blob/TAB, (b) I-C with T-blob/TTAB, (c) F-C with T-blob /TTAB

The fuel mass fraction contours for test case Y-1 are as indicated in figures 7.a and 7.b. The comparisons between figures 7.a and 7.b show that diffusion of the fuel species into the environment is at much lower rate than the case with the classical infinite conductivity model.

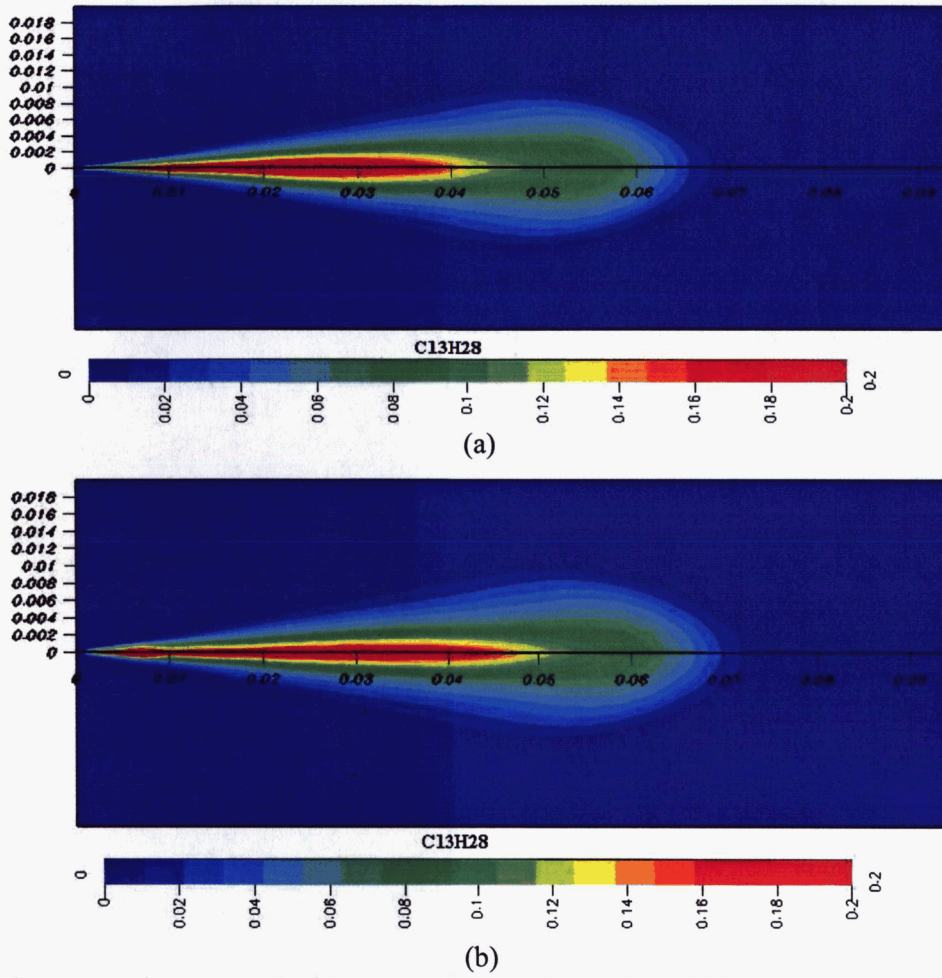


Figure 7. Fuel Mass Fraction Contours at 4 μ sec; (a) I-C with T-blob /TTAB, (b) F-C with T-blob/TTAB

4. Concluding Remarks

Based on the two-temperature film theory, a new finite-conductivity model accounting for droplet internal turbulence effect is developed for evaporating spray numerical calculations. The model is an extension of the existing T-blob/T-TAB atomization/spray model which provides the turbulence characteristics for estimating an effective thermal diffusivity within the droplet. Based on the one-way coupling simple spray results, the model exhibits reasonable physical trends in terms of droplets evaporation features. The current model can be efficiently incorporated into practical spray combustion CFD codes. In two-way Eulerian-Lagrangian multi-dimensional full CFD simulations utilizing CFD-ACE+ code, the current finite-conductivity model coupled with the T-blob/T-TAB model shows superior performance to the conventional infinite-conductivity evaporation model, by comparison to evaporating spray experimental data.

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