Direct Numerical Simulation of a Temporal Mixing Layer Laden with Multicomponent Evaporating Droplets

EXTENDED ABSTRACT

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May 4, 2001

1   NOTATION

B	transfer number: $\frac{y_s - y_g}{1 - y_s}$	**Greek letters**	
D	droplet diameter (m)	α, β	distribution parameters
Cp	heat capacity at ambient pressure	γ	distribution origin
e_t	total energy: kinetic energy+ internal energy	Γ	Fickian diffusion coefficient (m^2/s)
I	distribution variable: species molecular weight	θ	distribution meanmolecular mass
J_i	mass flux	λ	gas thermal conductivity (W/mK)
m	mass (kg)	ρ	mass density (kg/m^3)
R	gas constant/molar weight	τ_{ij}	viscous stress tensor
Re_b	blowing Reynolds number	χ	mol fraction
Re_d	dropelt Reynolds number based on slip velocity	ψ	distribution second central moment
Pr	Prandtl number		
Nu	Nusselt number		
Sc	Schmidt number	**Subscripts**	
Sh	Sherwood number	d	droplet
P	gas pressure (Pas)	G	gas
T	temperature (K)	L	liquid
u_i	gas velocity (m/s)	s	droplet surface
v_i	droplet velocity (m/s)	v	vapor
X_i	droplet position		
Y	mass fraction		

2 INTRODUCTION

Most combustion devices use fuel sprays utilizing commercial petroleum typically containing hundreds of pure species. The modeling of such spray flows is currently a subject of research. However, the physical phenomena involved in combustion chamber complex flows can be studied in simpler configurations such as mixing layers. For example, Direct Numerical Simulations of temporal mixing layer laden with single component droplets were presented in Miller and Bellan (1999)[3] and Okong'o and Bellan (2000)[6]. The purpose of the present study is to highlight the influence of real fuel droplets on the general mixing layer characteristics.

Complex multicomponent mixtures cannot be modeled by accounting for each single constituent; instead they are traditionally modeled using pseudo-component methods. Cotterman, Bender and Prausnitz (1985)[7] have proven the better suitability of Continuous Thermodynamics for performing phase equilibrium calculation such as the quasi-steady evaporation of droplets. Continuous distribution density functions are used instead of the mole fractions of individual components, or pseudo-components for describing the composition of those complex mixtures. Based on this approach, Tamin and Hallett (1995)[8] and Hallett (2000)[2], have developed a simple model for the vaporization of droplets with very many components. This model is now implemented in the context of Direct Numerical Simulation (DNS) of a Eulerian-Lagrangian two-phase turbulent flow with a large number of droplets, taking into account the momentum transfer related to drag forces, and the energy and mass transfers related to the evaporation.

3 MATHEMATICAL MODEL

The governing equations describe the Lagrangian transport of discrete evaporating droplets of a fuel mixture through a continuous and calorically perfect compressible gas flow. Instead of using as many transport equations as species involved in the mixture, the fuel composition (under liquid and vapor phases) is described using a two-parameter distribution function. The distribution function, $f(I)$ is so defined that

$$y_i = f(I)_i \Delta I_i$$

is the mol fraction of species i whose characterization index I lies within the small range I to $I + \Delta I$. In our particular case the distribution variable I is the molecular weight. Whitson (1983) has shown how gamma distributions may be used to characterize the high molecular-weight portion of crude oils. Γ distributions are thus selected for both gas and liquid and have the following general expression:

$$f(I) = \frac{(I - \gamma)^{\alpha - 1}}{\beta^\alpha \Gamma(\alpha)} \exp\left[-\left(\frac{I - \gamma}{\beta}\right)\right].$$

The vapor is present with overall mol fraction y_v, the remainder being air so that $y_a = 1 - y_v$, and in the vapor phase, the species mol fraction becomes

$$y_i = y_v f(I)_i \Delta I_i \qquad (1)$$

Additionally to the equations for the gas phase described in Miller and Bellan (1999)[3], two transport equations for the distribution function mean (θ) and second moment (ψ) also need to be solved as described in Tamin and Hallett (1995)[8]. Those two last transport equations are obtained by substituting Eq.(1) and that same equation weighted by I, into the species transport equation and then by integrating over the whole mixture. For the purpose of two-way coupled DNS, source terms describing the phase coupling of mass, momentum, energy and composition are also added to the system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j\right] = S_I$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_i u_j + P\delta_{ij} - \tau_{ij}\right] = S_{II,j}$$

$$\frac{\partial (\rho e_t)}{\partial t} + \frac{\partial}{\partial x_j}\left[\left(\rho e_t + P\right)u_j - \lambda\frac{\partial T}{\partial x_j} - u_i\tau_{ij} + \sum_{k=\text{species}} J_{jk}h_k\right] = S_{III}$$

$$\frac{\partial (\rho y_v)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho y_v u_j - \rho\Gamma\frac{\partial y_v}{\partial x_j}\right] = S_I$$

$$\frac{\partial (\rho y_v \theta_v)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho y_v \theta_v u_j - \rho\Gamma\frac{\partial (y_v\theta_v)}{\partial x_j}\right] = S_{IV}$$

$$\frac{\partial (\rho y_v \psi_v)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho y_v \psi_v u_j - \rho\Gamma\frac{\partial (y_v\psi_v)}{\partial x_j}\right] = S_V$$

$$P = \rho\left[y_v R_v + (1 - y_v) R_c\right] T$$

Coupled to the gas phase conservation equations, the Lagrangian particle equations for the position, the velocity, the temperature, the liquid distribution function mean molecular weight and the liquid distribution function second moment are respectively

$$\frac{dX_i}{dt} = v_i$$

$$\frac{dv_i}{dt} = \frac{F_i}{m_d}$$

$$\frac{dT_d}{dt} = \frac{Q + \frac{dm_d}{dt}L_v}{m_d C_L}$$

$$\frac{d\theta_L}{dt} = \frac{6J_{sm}}{\rho_L D}\left[\theta_L + \frac{\theta_v y_v - \theta_{vs} y_{vs}(1+B)}{B}\right]$$

$$\frac{d\psi_L}{dt} = \frac{6J_{sm}}{\rho_L D}\left[\psi_L + \frac{\psi_v y_v - \psi_{vs} y_{vs}(1+B)}{B}\right]$$

where the force terms F_i, the heat transfer terms Q, and the single droplet evaporation rate term $\frac{dm_d}{dt}$ or the mass flux at droplet's surface J_{sm} take into account the coupling between the flow and the droplets. Knowing the gas phase variables (u_i, T, y_v, P) at the droplet location, and using the validated models for the drag force F_i, the heat flux Q and the evaporation rate $\frac{dm_d}{dt}$ described in Miller, Harstad and Bellan (1998) we obtain:

$$F_i = m_d\left(\frac{f_1}{\tau_d}\right)(u_i - v_i)$$

$$Q = m_d\left(\frac{f_2}{\tau_d}\right)\left(\frac{NuC_{p,G}}{3\,\mathrm{Pr}}\right)(T - T_d)$$

$$\frac{dm_d}{dt} = -m_d\left(\frac{1}{\tau_d}\right)\left(\frac{Sh}{3Sc}\right)\ln(1+B)$$

f_1 is an empirical correction to Stokes drag accounting for finite droplet Reynolds numbers (Re_d):

$$f_1 = \frac{1 + 0.054\,\mathrm{Re}_d + 0.1\,\mathrm{Re}_d^{1/2}(1 - 0.03\,\mathrm{Re}_d)}{1 + a\,|\mathrm{Re}_b|^b}$$

$$a = 0.09 + 0.077\exp(-0.4\,\mathrm{Re}_d)$$

$$b = 0.4 + 0.77\exp(-0.04\,\mathrm{Re}_d)$$

f_2 is an analytical evaporative heat transfer correction

$$f_2 = \frac{\beta}{\exp(\beta) - 1}$$

$$\beta = -1.5\,\mathrm{Pr}\,\tau_d\frac{dm_d}{dt}/m_d$$

The source terms for the mean and second moment of the distribution function follow also the general form adopted in Miller and Bellan (1999)[3]:

$$S_I = -\sum_\alpha \left(\frac{w_\alpha}{\Delta x^3} \left[\frac{dm_d}{dt} \right]_\alpha \right)$$

$$S_{II,i} = -\sum_\alpha \left(\frac{w_\alpha}{\Delta x^3} \left[F_i + \frac{dm_d}{dt} v_i \right]_\alpha \right)$$

$$S_{III} = -\sum_\alpha \left(\frac{w_\alpha}{\Delta x^3} \left[v_i F_i + Q + \frac{dm_d}{dt} \left(\frac{v_i v_i}{2} + h_{v,s} \right) \right]_\alpha \right)$$

$$S_{IV} = -\sum_\alpha \left(\frac{w_\alpha}{\Delta x^3} \left[\frac{dm_d}{dt} \theta_v \right]_\alpha \right)$$

$$S_V = -\sum_\alpha \left(\frac{w_\alpha}{\Delta x^3} \left[\frac{dm_d}{dt} \psi_v \right]_\alpha \right)$$

where the summations are over local individual droplet contributions and a geometrical weighting factor w_α has been used to distribute the individual contributions to the nearest grid points. Evaluation of thermophysical properties is performed by using composition dependent correlations of Tamin and Hallett (1995)[8] and Chou and Prausnitz (1986)[1].

4   NUMERICAL PROCEDURE

The governing equations are solved numerically using fourth-order explicit Runge-Kutta temporal integration for all time derivatives and eight-order central finite differences for all spatial derivatives. A fourth-order Lagrange interpolation procedure is used to obtain gas phase variable values at droplet locations.

5   RESULTS

5.1   Single droplet, single component

First, the multicomponent model is used in the particular case of a pure component droplet: n-decane. Comparing evaporation behavior with those experimental and numerical results analyzed in Miller, Harstad and Bellan (1998)[5] for the purpose of evaporation models evaluation provide us with some validated results which can lead us then to study more complex mixtures for which experimental data are seldom detailed in the literature.

5.2   Single droplet, multicomponent

The graphs plotted on Fig. 1 show first (a) the evolution of the normalized droplet square diameter. For a heavy fuel such as diesel, which is not as

volatile as gasoline for example, even though the temperature gradient is high ($T_G = 1000$ K, $T_d = 300$ K) a heating period is still needed before the vaporization process starts. Droplet lifetime results can be sensibly different from one study to the other. This shows how temperature evolution and evaporation are highly dependent on transport and other thermophysical properties of liquid and vapor mixtures. Then, although the surface vapor mass fraction for the present model reaches an asymptote (see graph c) corresponding to quasi-steady evaporation, the droplet temperature (see graph b) does not reach such an asymptotic state (as in the case of single component droplet) because the composition of the droplet changes which indeed modifies the boiling temperature. The last graph (d) shows how the liquid composition evolves during the evaporation. Half way of the droplet lifetime, the distribution function modeling the liquid phase composition narrows. Actually, as expected, the lighter components evaporate first while the heavier ones are vaporized by the end of droplet's lifetime. Moreover, the variation in the liquid composition leads to a variation in the vapor composition around the droplet which affects the evaporation process and modifies the thermophysical properties.

5.3 Temporal mixing layer laden with fuel droplets

The simulation of the mixing layer is conducted within the same domain and configuration as previous studies of Miller and Bellan (1999, 2000) [3],[4] and Okong'o and Bellan (2000)[6] where single component droplets were used. The multicomponent droplet model and transport equations related to that model enable us to highlight the influence of the heterogeneous vapor composition and variable droplet thermophysical properties on the mixing layer growth rate and kinetic energy. Furthermore, it is interesting to analyze the vapor composition field and relate it to the droplet evaporation history and vorticity region locations in the numerical domain. Such a systematic investigation will be presented in the paper.

6   CONCLUSION

The influence of the multicomponent aspect of the fuel drops has been here studied in a mixing layer configuration. Results highlighting the difference between single and multicomponent drop simulations in the same geometric configuration will be discussed.
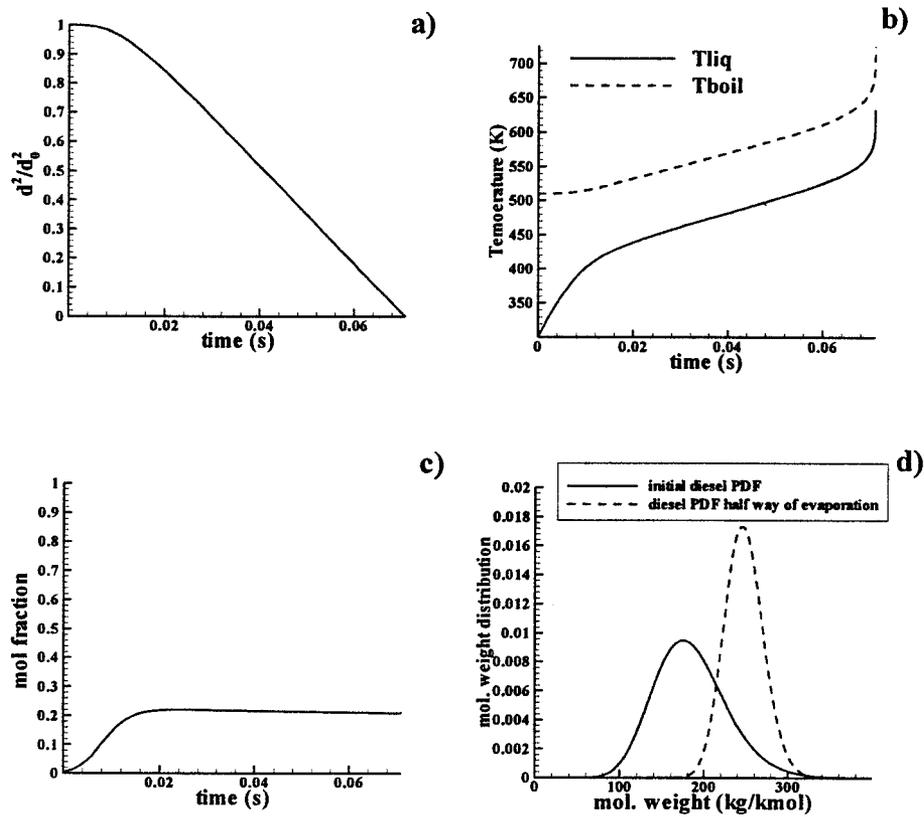
Figure 1: Quiescent diesel droplet evaporation. Initial droplet temperature: 300 K. Initial gas temperature: 1000 K. Initial dropelt diameter: $100\,\mu m$.

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