SIMPLE MODEL OF TRANSIENT DROP VAPORIZATION

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Abstract

A new drop vaporization model incorporating the effects of transient heat and mass transfer between drop and gas is presented. The model is based on two ordinary differential equations with the correction function obtained from the analytical solution of the heat conductivity equation and is valid for arbitrary Lewis numbers. The model has been validated against the numerical solution of the transient conjugate problem of drop vaporization with regard for multicomponent diffusion for several primary reference hydrocarbons (n-heptane, n-decane, n-dodecane, and n-tetradecane) at the gas temperature ranging from 400 to 1500 K and pressure from 1 to 40 MPa. Comparison of the new model performance with a standard drop vaporization model used in commercial CFD codes is made within the same ranges of gas temperature and pressure. The new model was shown to provide more realistic characteristic times of drop heating and vaporization.

Keywords: solid particle, transient heating, metal particle ignition, mathematical model.

1. Introduction

For multidimensional simulation of fuel sprays in power plants and engines, simple models of drop heating and vaporization providing adequate rates of interphase heat and mass exchange are required. Available simple drop heating and vaporization models (see, e.g., [1–4]) exhibit several drawbacks. One of them is the application of Newton’s law for the heat flux at the drop surface. Newton’s law is known to be applicable to steady-state rather than transient heat transfer. Therefore special “corrections” should be used to justify its application. In the simple drop heating models, the drop energy balance equation reads

\[ m_d c_\ell \frac{dT_d}{dt} = \dot{Q} + \frac{dm_d}{dt}, \]

where \( m_d = \frac{4}{3} \pi r_d^3 \rho_\ell \) is the drop mass, \( c_\ell \) is the specific heat of liquid, and \( \rho_\ell \) is the liquid density. The total heat flux is usually determined from Newton’s law

\[ \dot{Q} = A_d q = A_d \alpha (T_g - T_d), \]

where

\[ q = \alpha (T_g - T_d) \]

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is the heat flux per unit surface area of the drop and \( A_d = 4\pi r_d^2 \) is the spherical drop surface area. In Eq. (2) \( \alpha \) is the heat transfer coefficient, \( T_d \) is the mean drop temperature, and \( T_g \) is the gas temperature at a sufficiently large distance from the drop. In the absence of gas flow (zero Reynolds number), the Nusselt number \( \text{Nu} \approx 2 \) and one obtains a simple expression for the heat transfer coefficient \( \alpha \)

\[
\alpha = \frac{\alpha_g}{r_d},
\]

where \( \alpha_g \) is the gas heat transfer coefficient. Equation (3) is valid, strictly speaking, only for stationary cases. Nevertheless, it is widely used for modeling both stationary and transient processes, including vaporization and combustion of fuel drops. The applicability of Eq. (3) to transient processes has not been rigorously justified so far.

In [5], the transient heat transfer between a spherical body and surrounding gas was investigated to clarify the range of applicability of Eqs. (3) and (4). In the analysis of [5], constant-temperature boundary conditions were applied at the drop surface. The analytical solution of the thermal conductivity equation for this case is given by

\[
T = T_g + \frac{r_d}{r} (T_{ds} - T_g) \left[ 1 - \text{erf} \left( \frac{r - r_d}{2 \sqrt{\lambda_g t / \rho_g c_{pg}}} \right) \right],
\]

where

\[
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz,
\]

\( r \) is a radial coordinate, \( t_{ds} \) is the drop surface temperature, \( \lambda_g \) is the gas thermal conductivity, \( \rho_g \) is the gas density, and \( c_{pg} \) is the gas specific heat at a constant pressure. Based on Eq. (5), the following expression for the transient heat flux at the drop surface was derived in [5]:

\[
q = \lambda_g \frac{\partial T}{\partial r} = \lambda_g \frac{T_g - T_{ds}}{r_s} \left( 1 + \frac{r_d}{\sqrt{\pi \lambda_g t / \rho_g c_{pg}}} \right).
\]

When comparing Eq. (7) with Eqs. (3) and (4), Newton’s law (3) with the condition (4) can be used for modeling the transient heat transfer, if the actual thermal conductivity of gas \( \lambda_g \) is replaced by the “effective” thermal conductivity \( \lambda_{\text{eff}} \) given by the equation

\[
\lambda_{\text{eff}} = \lambda_g (1 + \varphi),
\]

where

\[
\varphi = r_d \sqrt{\frac{\rho_g c_{pg}}{\pi \lambda_g t}}.
\]

On the one hand, in the limit \( t \rightarrow \infty \), \( \lambda_{\text{eff}} \rightarrow \lambda_g \), as could be expected. On the other hand, \( \lambda_{\text{eff}} \rightarrow \infty \) at \( t \rightarrow 0 \). The latter implies that the transient initial stage of the drop heating can play an essential role in the drop-temperature evolution. This result was applied for the description of the fuel drop heating in a medium duty truck Diesel engine in [5] where it has been shown that for adequate application of Newton’s law (3) the gas thermal conductivity \( \lambda_g \) may need to be increased by more than 100% for the initial stages of calculations to account for transient effects during drop heating. In this paper, a new model of the drop vaporization is suggested to account for the transient heating effects discussed in [5].
2. Approach

2.1. New Model of Drop Vaporization

The new model is based on the equations and relationships given below:

Equation of drop heating (1);
Equation (2) for heat flux at the drop surface;
The equation of drop vaporization
\[
\frac{dm_d}{dt} = -\pi d^2 j, \quad (10)
\]
where \(d\) is the drop diameter and \(j\) is the liquid vapor mass flow rate due to evaporation at the drop surface;

The equation for the heat transfer coefficient [4]
\[
\alpha = \frac{Nu}{d} \frac{\lambda_{\text{eff}} \ln(1 + B)}{B}, \quad (11)
\]
where \(\ln(1 + B)/B\) is the Spalding heat-transfer modification function, with \(B\) being the mass transfer number;

The equation for liquid vapor mass flow rate
\[
j = 2 \frac{\rho_g D}{d} \ln(1 + B); \quad (12)
\]

The equation for the mass transfer number
\[
B = \frac{Y_{vs} - Y_{v\infty}}{1 - Y_{vs}}, \quad (13)
\]
where \(Y_v\) is the mass fraction of liquid vapor, and indices \(s\) and \(\infty\) denote the drop surface and a large distance from the drop;

The equation for the Nusselt number [6, 7]
\[
Nu = 2 + 0.6 \frac{Re^{1/2} Pr^{1/3} j}{}, \quad (14)
\]
where \(Re\) is Reynolds number and \(Pr\) is Prandtl number.

Equation (8) for the effective thermal conductivity \(\lambda_{\text{eff}}\);

The equation for the \(\varphi\)-function [similar to Eq. (9)]
\[
\varphi = \beta r_d \sqrt{\frac{\rho g c_{pg}}{\pi \lambda g}}, \quad (15)
\]
where \(\beta\) is the correction factor with the default value of \(\beta = 1.0\);

All liquid properties are taken as functions of the mean liquid temperature, i.e.,
\[
\rho_\ell = \rho_\ell(T_d), \quad c_\ell = c_\ell(T_d); \quad (16)
\]

All gas properties in the film near the drop surface are taken at the mean drop temperature, i.e.,
\[
\lambda_g = \lambda_g(T_d, p), \quad c_{pg} = c_{pg}(T_d), \quad D = D(T_d, p); \quad (17)
\]
The equation for the gas density (the ideal-gas equation of the state)

\[ \rho_g = \frac{p\bar{W}}{RT_g}, \]  

(18)

where \( p \) is pressure, \( \bar{W} \) is the mean molecular mass of gas mixture, and \( R \) is the universal gas constant.

The equation for the mean molecular mass

\[ W = \frac{1}{\sum_{j=1}^{N} Y_i/W_i}; \]  

(19)

The initial condition for Eq. (1)

\[ T_d(0) = T_{d0}; \]  

(20)

The initial condition for Eq. (10)

\[ m_d(0) = m_{d0}, \]  

(21)

where \( m_{d0} = (4/3)\pi r_{d0}^3 \rho_l \) is the initial drop mass.

The model based on Eqs. (1), (2), and (10)--(21) does not apply the assumption on the unity Lewis number and does not apply the concept of “reference” temperature usually used in simple models of drop vaporization. In addition, it takes into account transient heat transfer between gas and drop by introducing the time-dependent correction function \( \varphi(t) \) [see Eq. (15)]. Also, it provides a possibility of introducing a user-defined correction coefficient \( \beta \) to improve the model performance. Introducing the correction coefficient \( \beta \) is physically justified due to the origin of function \( \varphi(t) \). Recall that the exact expression for \( \varphi(t) \) is obtained from the solution of the heat conductivity equation at a constant drop-surface temperature. If the drop-surface temperature varies with time, the expression for \( \varphi(t) \) should be modified in general. Note that the model described herein does not take into account the difference between the mean and surface temperature of the drop.

2.2. Detailed Model of Drop Evaporation

For validating the new drop vaporization model, a detailed model of drop vaporization solving the conjugate problem of heat and mass transfer of a spherical fuel drop with the ambient gas (forced and natural convection is not taken into account) was used. Below, the mathematical statement of the problem is described [8, 9].

The equation for the drop mass evolution reads

\[ \frac{m_d}{dt} = 4\pi r_{d}^2 \rho_{ls} u_s, \]  

(22)

where \( \rho_{ls} \) is the liquid density at the drop surface and \( u_s = u_s(t) \) is the drop surface velocity component due to liquid vaporization. Note that there exists another component of the drop velocity caused by liquid expansion.

The initial condition for Eq. (22) reads

\[ m_d(0) = m_{d0}. \]  

(23)
The thermal conductivity equation in the drop \((0 < r < r_d)\) is

\[
c_\ell \rho_\ell \frac{\partial T_\ell}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( \lambda_\ell r^2 \frac{\partial T_\ell}{\partial r} \right),
\]

where \(r\) is the radial coordinate, \(t_\ell\) is the liquid temperature depending on the radial coordinate and time, i.e., \(T_\ell = t_\ell(r, t)\), \(c_\ell(T_\ell)\) is the liquid specific heat, \(\rho_\ell(T_\ell)\) is the liquid density, and \(\lambda_\ell(T_\ell)\) is the liquid thermal conductivity.

The initial condition for Eq. (24) is

\[
T_\ell(0, r) = T_{\ell 0}.
\]

The boundary condition for Eq. (24) in the drop center \((r = 0)\) is

\[
\frac{\partial T_\ell}{\partial r} = 0.
\]

The boundary conditions for Eq. (24) at the drop surface \((r = r_d)\) is

\[
T_\ell = T_g.
\]

The equation for the vapor mass fraction at the drop surface \((r = r_d)\) reads

\[
Y_v = \frac{p_v}{p} \frac{W_v}{W},
\]

where \(p_v\) is the vapor pressure at the drop surface and \(W_v\) is the molecular mass of vapor.

The continuity equation in the gas phase \((r_d < r < \infty)\) reads

\[
\frac{\partial \rho_g}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_g u_g \right) = 0,
\]

where \(u_g\) is the gas velocity.

The initial condition for Eq. (29) reads

\[
\rho_g(0, r) = \rho_{g 0},
\]

where \(\rho_{g 0}\) is taken uniformly distributed in the gas phase.

The boundary condition for Eq. (29) at the drop surface \((r = r_d)\) is

\[
-\rho_\ell u_s = \rho_g \left( u_g - \frac{\partial r_d}{\partial t} \right),
\]

where the derivative \(\partial r_d/\partial t\) is the instantaneous velocity of the drop surface due to both thermal expansion and vaporization.

The species continuity equations in the gas phase \((r_d < r < \infty)\) reads

\[
\rho_g \frac{\partial Y_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_g Y_i V_i \right) - \rho_g u_g \frac{\partial Y_g}{\partial r},
\]

where \(Y_i\) is the mass fraction of the \(i\)th species in the gas phase, \(V_i\) is the diffusion velocity of the \(i\)th species, and \(Y_g\) is the gas mass fraction.
Equation for species diffusion velocities in the gas phase \((r_d < r < \infty)\) is

\[
\frac{\partial X_i}{\partial t} = \sum_{j=1}^{N} \left( \frac{X_i X_j}{D_{ij}} \right) (V_j - V_i),
\]

(33)

where \(X_i = Y_i \bar{W}/W_i\) is the molar fraction of the \(i\)th species and \(D_{ij}\) is the binary diffusion coefficient of species \(i\) and \(j\) in a multicomponent gas mixture.

The initial condition for Eq. (32) is

\[
Y_i(0, r) = Y_{i0}, \quad i = 1, 2, \ldots, N,
\]

(34)

where \(Y_{i0}\) is taken uniformly distributed in the gas phase.

The boundary condition for Eq. (32) at the drop surface \((r = r_d)\) is

\[
-\rho \ell us \beta_i = \rho_g \left( u_g - Y_i \frac{\partial r_d}{\partial t} \right) + \rho_g Y_i V_i,
\]

(35)

where

\[
\beta_i = 1 \quad \text{at} \quad i = v \quad \text{and} \quad \beta_i = 0 \quad \text{at} \quad i \neq v.
\]

The boundary conditions for Eq. (32) at a far distance from the drop surface \((r \to \infty)\) are

\[
\frac{\partial \bar{W}Y_i}{\partial r} = 0, \quad i = 1, 2, \ldots, N.
\]

(36)

The energy conservation equation for the gas phase \((r_d < r < \infty)\) reads

\[
c_{pg} \rho_g \frac{\partial T_g}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \lambda_g \frac{\partial T_g}{\partial r} \right) - c_{pg} \rho_g \bar{u}_g \frac{\partial T_g}{\partial r},
\]

(37)

where \(c_{pg} = c_{pg}(T_g)\), \(\rho_g = \rho_g(p, T_g)\), and \(\lambda_g(p, T_g)\) are the specific heat, density, and thermal conductivity of the gas.

The boundary condition for Eq. (37) at the drop surface \((r = r_d)\), which is similar to Eq. (27), reads

\[
T_g = T_\ell.
\]

(38)

The boundary conditions for Eq. (37) at a far distance from the drop surface \((r \to \infty)\) is

\[
\frac{\partial T_g}{\partial r} = 0.
\]

(39)

The Tailoring boundary condition for Eqs. (24) and (37) at the drop surface \((r = r_d)\) required for determining the problem eigenvalue \(T_{ds}\)

\[
\lambda_\ell \frac{\partial T_\ell}{\partial r} - \frac{\rho_\ell us L_s}{W_v} = \lambda_g \frac{\partial T_g}{\partial r}.
\]

(40)

The ideal gas equation of state (18) for the gas phase is used along with the constant pressure condition

\[
p = p_0,
\]

(41)

where \(p_0\) is a constant taken throughout the entire vaporization process.
Fig. 1. Comparison of predicted (curves) and measured (points) dynamics of \(n\)-heptane (a) and \(n\)-tetradecane (b) drop surface regression at vaporization in air, \(d_0 = 70 \mu m\), \(T_{\ell 0} = 293.15 K\), and \(T_g0 = 573.15 K\) [8–10].

3. Results

3.1. Comparison with Experimental Data

Equations (22)–(41) were solved numerically with continuous monitoring of the material and energy balance between liquid and gas phases. A detailed description of the numerical procedure is given in [8, 9]. To validate the detailed model, multiple comparisons have been made with available experimental data (see [8–10]). The predicting capability of the detailed model is demonstrated by Fig. 1 where predicted and measured drop surface regression curves for \(n\)-heptane (Fig. 1a) and \(n\)-tetradecane (Fig. 1b) drops of initial diameter \(d_0 = 70 \mu m\) at air temperature \(T_g0 = 573\) and pressure \(p = 0.1 \text{ MPa}\) are compared.

In the simplest standard model of drop vaporization based on the quasisteady vaporization law, the dependence \(d^2(t)\) is known to be linear. In the detailed model, this dependence is more complicated — due to liquid transient heating and thermal expansion the \(d^2(t)\) function exhibits a nonlinear behavior. The detailed model is seen to provide good predictions for liquid drops evaporating at microgravity conditions. Note that the detailed model presented above does not contain any fitting parameter.

4. “Wet Bulb” Temperature

When the mean drop temperature \(T_d\) attains the value of saturation temperature (“wet bulb” temperature) \(T_{ds} = T_{wb}\), the heat flux to the drop interior vanishes, i.e., \(dT_d/dt = 0\), and the entire heat flux \(\dot{Q}\) is consumed for liquid vaporization. The initial period in the drop evolution, when \(dT_d/dt \neq 0\) or \(T_d < T_{wb}\), is usually referred to as the transient heating period. Its duration will be denoted by \(t_h\). The period when \(dT_d/dt = 0\) or \(T_d = T_{wb}\) is referred to as the period of quasisteady drop vaporization. In the latter case, instead of Eq. (1) one can write

\[
t_d = T_{ds} = T_{wb}
\]
Fig. 2. Predicted time histories of surface (solid curves) and mean (dashed curves) temperature of a vaporizing n-heptane drop 50 μm in diameter at $T_{d0} = 293$ K and $p = 0.1$ MPa with $T_g = 1000$ K (a) and 1500 K (b). Dash-and-dot lines correspond to “wet bulb” temperature found from Eq. (44).

and

$$\dot{Q} = -L \frac{dm_d}{dt}. \quad (43)$$

The “wet bulb” temperature $T_{wb}$ can be found based on the simple model described in Sec. 1.1 and based on the detailed model of Sec. 1.2. Substituting Eqs. (10)–(14) into Eq. (43) gives the following relationship for $T_{ds} = T_{wb}$:

$$Nu \lambda_g (T_g - T_i) = 2 \rho_g DL \frac{Y_{vi} - Y_{v\infty}}{1 - Y_{vi}}. \quad (44)$$

In Eq. (44), the parameters $\lambda_g$, $\rho_g$, $D$, $L$, and $Y_{vi}$ are functions of temperature $T_{ds}$, therefore, the solution of Eq. (44) should be found by iteration. To check the validity of Eq. (44), we have performed detailed numerical calculations of spherical drop heating and vaporization using the model of Sec. 1.2.

The solid and dashed curves in Fig. 2a and b show the predicted dynamics of surface temperature $T_{ds}$ and mean temperature $T_d$ for an n-heptane drop at $T_{d0} = 293$ K, pressure $p = 0.1$ MPa, and two values of gas temperature $T_g = T_{g\infty} = 1000$ and 1500 K. Horizontal dash-and-dot lines correspond to the solution of Eq. (44) at $Nu = Nu_{sq} = 2$. Figure 3 shows similar results for the evaporating n-dodecane drop. Termination of the curves in Figs. 2 and 3 corresponds to the complete drop vaporization (lifetime $t_\ell$).

Analysis of Figs. 2 and 3, as well as the results of calculations at other values of $T_g$ and $p$ and for other liquids, results in the following conclusions:

1. The time taken for the drop surface temperature $T_{ds}$ to attain a value close to the “wet bulb” temperature $T_{wb}$ is considerably smaller than the total drop lifetime, in particular, at high gas temperatures $T_g$. This observation justifies the use of the exact expression for $\varphi(t)$ obtained from the solution of
Fig. 3. Predicted time histories of surface (solid curves) and mean (dashed curves) temperatures of a vaporizing $n$-dodecane drop $50 \, \mu m$ in diameter at $T_{d0} = 293 \, K$ and $p = 0.1 \, MPa$ with $T_g = 1000 \, K$ (a) and $1500 \, K$ (b). Dash-and-dot lines correspond to “wet bulb” temperature found from Eq. (44).

the heat conductivity equation at a constant drop-surface temperature and the default value of $\beta = 1.0$ in the model of Sec. 1.1.

(2) At high gas temperatures, the duration of the transient heating period $t_h$ is comparable with the total drop lifetime $t_\ell$.

(3) Equation (44) resulting from the simplified model of Sec. 1.1 provides a good estimate for the “wet bulb” temperature $T_{wb}$ in a wide range of gas temperatures and pressures, as well as physical properties of the liquid. If the drop is placed in the gas flow, the values of wet-bulb temperature will be somewhat different from the value relevant to drop vaporization in a quiescent atmosphere. This is evident from Eq. (44). At $Re_g \neq 0$, the Nusselt number in Eq. (44) can be estimated based on Eq. (14) for a spherical drop.

4.1. Simple Model Performance

The new vaporization model of Sec. 1.1 was compared with the Dukowicz model [2], which is often used in commercial CFD codes, and with the detailed model of Sec. 1.2 for a ambient gas (air) pressure ranging from 1 to 40 bar and for a gas temperature ranging from 400 to 1500 K. Drops of different primary reference hydrocarbon fuels were considered, namely, $n$-heptane, $n$-decane, $n$-dodecane, and $n$-tetradecane. Only some results for $n$-heptane drops are presented herein. The results of model comparisons for other hydrocarbons are very similar to those relevant to $n$-heptane drops. The initial diameter and temperature of $n$-heptane drops were taken equal to $50 \, \mu m$ and $293 \, K$, respectively. The correction factor $\beta$ [see Eq. (15)] was not varied in the calculations and was taken equal to 1.0.

Figures 4 and 5 show the comparison of the Dukowicz model (dashed curves) with the new model (solid curves) and detailed model (dotted curves) for a pressure of 1 bar and temperatures of 800 and 1200 K. It is seen from Figs. 4 and 5 that the new vaporization model predicts correctly the drop
5. Concluding Remarks

Validation of the new drop vaporization model against the detailed model indicates that the former provides a good prediction in terms of the “wet bulb” temperature and drop lifetime within a wide range of gas temperatures and pressures. In the case where the new-model based solution is somewhat different from the exact solution, the drop lifetime is usually slightly overestimated. Therefore the correction coefficient $\beta$ [see Eq. (15)] could be taken a bit larger than 1.0 for a better prediction of the drop lifetime. In general, the new model provides much better results than the Dukowicz model, which is often used in commercial CFD codes. The latter underestimates systematically the “wet bulb” temperature and the predicted drop lifetime is, as a rule, shorter than that predicted by the detailed solution by a factor of 1.5 to 3.
Fig. 5. Vaporization of an n-heptane drop at $T_{g0} = 1200$ K, $p = 1$ bar, and $T_{00} = 293$ K for mean temperature (a) and drop diameter histories (b).

Fig. 6. Vaporization of an n-heptane drop at $T_{g0} = 800$ K, $p = 10$ bar, and $T_{00} = 293$ K for mean temperature (a) and drop diameter histories (b).
Fig. 7. Vaporization of an n-heptane drop at $T_{g0} = 1200 \text{ K}$, $p = 10 \text{ bar}$, and $T_{l0} = 293 \text{ K}$ for mean temperature (a) and drop diameter histories (b).

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