

MATHEMATICAL MODEL FOR TRANSIENT DROPLET VAPORIZATION

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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 heat conductivity equation and is valid for arbitrary Lewis numbers. The model has been validated against the numerical solution of the nonstationary conjugate problem of drop vaporization with regard for multicomponent diffusion for three primary reference hydrocarbons (*n*-heptane, *n*-octane, and *n*-dodecane) at gas temperatures ranging from 400 to 1500 K and pressures from 1 to 40 bar. Only some results for *n*-heptane drops are presented herein. Comparison of the new model performance with a standard drop vaporization model used in commercial computational fluid dynamics (CFD) codes is made within the same ranges of gas temperature and pressure. It has been shown that the new model provides more realistic characteristic times of drop heating and vaporization.

Nomenclature

A_d drop surface area, m²
 a temperature diffusivity coefficient, m²/s
 B mass transfer number
 c_l specific heat of liquid, J/(kg·K)
 $c_{p,g}$ gas specific heat at constant pressure, J/(kg·K)

D	binary diffusion coefficient, m ² /s
D_{ij}	binary diffusion coefficient of species i and j in a multicomponent gas mixture, m ² /s
d	drop diameter, m
j	liquid vapor mass flow rate due to vaporization at the drop surface, kg/(m ² ·s)
L	latent heat of vaporization, J/kg
L_s	latent heat of vaporization at drop surface temperature T_s , J/kg
m_d	drop mass, kg
m_{d0}	initial drop mass, kg
N	number of gaseous species
Nu	Nusselt number
\dot{Q}	total heat flux from the gas phase to a drop, W
p	pressure, Pa
p_0	initial pressure, Pa
p_v	vapor pressure at the drop surface, Pa
Pr	Prandtl number
q	heat flux per unit surface area of a drop, W/m ²
R	universal gas constant, J/(kmol·K)
r	radial coordinate, m
r_d	drop radius, m
r_{d0}	initial drop radius, m
Re	Reynolds number
T_d	mean drop temperature, K
T_{d0}	initial drop temperature, K
T_g	gas temperature, K
T_l	liquid temperature, K
T_{l0}	initial liquid temperature, K
t	time, s
u_g	gas velocity, m/s
u_s	drop surface velocity component due to liquid vaporization, m/s
V_i	diffusion velocity of the i th gaseous species, m/s
W	mean molecular mass of gas mixture, kg/kmol
W_i	molecular mass of the i th gaseous species, kg/kmol
X	molar fraction
Y	mass fraction
Y_v	vapor mass fraction
Y_{i0}	mass fraction of the i th gaseous species

Y_{i0}	mass fraction of the i th gaseous species
α	heat transfer coefficient, $W/(m^2 \cdot K)$
β	correction factor with the default value of 1.0
β_i	coefficient related to the i th gaseous species
λ_{eff}	effective thermal conductivity of gas, $W/(m \cdot K)$
λ_g	gas thermal conductivity, $W/(m \cdot K)$
λ_l	liquid thermal conductivity, $W/(m \cdot K)$
ϕ	equivalence ratio
φ	time-dependent correction function
ρ_l	liquid density, kg/m^3
ρ_g	gas density, kg/m^3
ρ_{g0}	initial gas density, kg/m^3
ρ_{l_s}	liquid density at drop surface temperature T_s , kg/m^3

Indices

0	relates to the initial value
d	relates to the drop
g	relates to the gas
i	relates to the i th gaseous species
j	relates to the j th gaseous species
l	relates to liquid
s	relates to the drop surface
v	relates to liquid vapor
∞	relates to large distance from the drop

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 [1–4] exhibit several drawbacks. One of them is the application of the Newton’s law for the heat flux at the drop surface. The 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.

This paper presents a new drop vaporization model incorporating the effects of transient heat and mass transfer between drop and gas.

Background

In the simple drop heating models, the drop energy balance equation reads

$$m_d c_l \frac{dT_d}{dt} = \dot{Q} + L \frac{dm_d}{dt} \quad (1)$$

where $m_d = (4/3)\pi r_d^3 \rho_l$ is the drop mass. The total heat flux is usually determined from the Newton's law:

$$\dot{Q} = A_d q = A_d \alpha (T_g - T_d) \quad (2)$$

where

$$q = \alpha (T_g - T_d) \quad (3)$$

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, α 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), $Nu = 2$ and one obtains a simple expression for α :

$$\alpha = \frac{\lambda_g}{r_d} \quad (4)$$

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:

$$T = T_g + \frac{r_d}{r} (T_{ds} - T_g) \left[1 - \operatorname{erf} \left(\frac{r - r_d}{2\sqrt{\lambda_g t / (\rho_g c_{pg})}} \right) \right] \quad (5)$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz \quad (6)$$

Based on Eq. (5), the authors of [5] derived the following expression for the transient heat flux at the drop surface:

$$q = \lambda_g \frac{\partial T}{\partial r} = \lambda_g \frac{T_g - T_{ds}}{r_s} \left(1 + \frac{r_d}{\sqrt{\pi \lambda_g t / (\rho_g c_{pg})}} \right) \quad (7)$$

When comparing Eq. (7) with Eqs. (3) and (4), one comes to a conclusion that the Newton's law (3) with the condition (4) can be used for modeling transient heat transfer if the actual thermal conductivity of gas λ_g is replaced with the 'effective' thermal conductivity λ_{eff} given by equation:

$$\lambda_{\text{eff}} = \lambda_g (1 + \varphi) \quad (8)$$

where

$$\varphi = r_d \sqrt{\frac{\rho_g c_{pg}}{\pi \lambda_g t}} \quad (9)$$

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 drop heating can play an essential role in drop temperature evolution.

The authors of [5] applied their finding for description of fuel drop heating in a medium duty truck Diesel engine. They have shown that for adequate application of the Newton's law (3), the gas thermal conductivity λ_g may need to be increased by more than 100% for the initial stages of calculations to account for transient effects during drop heating.

Approach

New Model of Drop Vaporization

In this paper, a new model of drop vaporization is suggested to account for the transient heating effects discussed in [5]. The model is based on the equations and relationships given below.

- Equation of drop heating (1);
- Equation (2) for heat flux at the drop surface;
- Equation of drop vaporization:

$$\frac{dm_d}{dt} = -\pi d^2 j \quad (10)$$

- Equation for the heat transfer coefficient:

$$\alpha = \frac{\text{Nu}}{d} \lambda_{\text{eff}} \frac{\ln(1+B)}{B} \quad (11)$$

where $\ln(1+B)/B$ is the Spalding heat-transfer modification function;

- Equation for liquid vapor mass flow rate:

$$j = 2 \frac{\rho_g D}{d} \ln(1+B) \quad (12)$$

- 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 ∞ stand for the drop surface and large distance from the drop;

- Equation for Nusselt number [6]:

$$\text{Nu} = 2 + 0.6\text{Re}^{1/2}\text{Pr}^{1/3} \quad (14)$$

- Equation (8) for the effective thermal conductivity λ_{eff} ;
- Equation for the φ -function (similar to Eq. (9)):

$$\varphi = \beta r_d \sqrt{\frac{\rho_g c_{pg}}{\pi \lambda_g t}} \quad (15)$$

where β 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.,

$$\rho_l = \rho_l(T_d), \quad c_l = c_l(T_d) \quad (16)$$

- All gas properties in the film near the drop surface are taken at the mean drop temperature, i.e.,

$$\lambda_g = \lambda_g(T_d, p), \quad c_{pg} = c_{pg}(T_d), \quad D = D(T_d, p) \quad (17)$$

- Equation for the gas density (ideal-gas equation of state):

$$\rho_g = \frac{pW}{RT_g} \quad (18)$$

- Equation for the mean molecular mass:

$$W = \frac{1}{\sum_{i=1}^N Y_i/W_i} \quad (19)$$

- Initial condition for Eq. (1):

$$T_d(0) = T_{d0} \quad (20)$$

- Initial condition for Eq. (10):

$$m_d(0) = m_{d0} \quad (21)$$

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

The model based on Eqs. (1), (2), (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 β to improve model performance. Introduction of the correction coefficient β is physically justified due

to the origin of function $\varphi(t)$. Remind that the exact expression for $\varphi(t)$ is obtained from the solution of the heat conductivity equation at constant drop-surface temperature. As the drop-surface temperature varies with time, the expression for $\varphi(t)$ should be modified. Note that the model described herein does not take into account the difference between the mean and surface temperature of the drop.

Detailed Model of Drop Vaporization

For validating the new drop vaporization model, a detailed model based on the conjugate equations of heat and mass transfer of 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 [7, 8].

- Equation for the drop mass:

$$\frac{dm_d}{dt} = 4\pi r_d^2 \rho_{l_s} u_s \quad (22)$$

where ρ_{l_s} 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 drop surface velocity caused by liquid thermal expansion.

- Initial condition for Eq. (22):

$$m_d(0) = m_{d0} \quad (23)$$

- Thermal conductivity equation in the drop ($0 < r < r_d$):

$$c_l \rho_l \frac{\partial T_l}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\lambda_l r^2 \frac{\partial T_l}{\partial r} \right) \quad (24)$$

where r is the radial coordinate, T_l is the liquid temperature depending on the radial coordinate and time, i.e., $T_l = T_l(r, t)$, $c_l(T_l)$ is the liquid specific heat, $\rho_l(T_l)$ is the liquid density, and $\lambda_l(T_l)$ is the liquid thermal conductivity.

- Initial condition for Eq. (24):

$$T_l(0, r) = T_{l0} \quad (25)$$

- Boundary condition for Eq. (24) in the drop center ($r = 0$)

$$\frac{\partial T_i}{\partial r} = 0 \quad (26)$$

- Boundary condition for Eq. (24) at the drop surface ($r = r_d$):

$$T_i = T_g \quad (27)$$

- Equation for vapor mass fraction at the drop surface ($r = r_d$):

$$Y_v = \frac{p_v}{p} \frac{W_v}{W} \quad (28)$$

- Continuity equation in the gas phase ($r_d < r < \infty$):

$$\frac{\partial \rho_g}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g u_g) = 0 \quad (29)$$

- Initial condition for Eq. (29):

$$\rho_g(0, r) = \rho_{g0} \quad (30)$$

where ρ_{g0} is taken uniformly distributed in the gas phase.

- Boundary condition for Eq. (29) at the drop surface ($r = r_d$):

$$-\rho_l u_s = \rho_g \left(u_g - \frac{\partial r_d}{\partial t} \right) \quad (31)$$

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

- Species continuity equations in the gas phase ($r_d < r < \infty$):

$$\rho_g \frac{\partial Y_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (\rho_g r^2 Y_i V_i) - \rho_g u_g \frac{\partial Y_i}{\partial r} \quad (32)$$

- Equation for species diffusion velocities in the gas phase ($r_d < r < \infty$):

$$\frac{\partial X_i}{\partial r} = \sum_{j=1}^N \left(\frac{X_i X_j}{D_{ij}} \right) (V_j - V_i) \quad (33)$$

where $X_i = Y_i W / W_i$ is the molar fraction of the i th species.

- Initial conditions for Eqs. (32):

$$Y_i(0, r) = Y_{i0} \quad i = 1, \dots, N \quad (34)$$

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

- Boundary conditions for Eqs. (32) at the drop surface ($r = r_d$):

$$-\rho_l u_s \beta_i = \rho_g \left(u_g - Y_i \frac{\partial r_d}{\partial t} \right) + \rho_g Y_i V_i \quad (35)$$

where

$$\begin{aligned} \beta_i &= 1 \text{ at } i = v \\ \beta_i &= 0 \text{ at } i \neq v \end{aligned}$$

- Boundary conditions for Eqs. (32) at far distance from the drop surface ($r \rightarrow \infty$):

$$\frac{\partial W Y_i}{\partial r} = 0, \quad i = 1, \dots, N \quad (36)$$

- Energy conservation equation for the gas phase ($r_d < r < \infty$):

$$c_{pg} \rho_g \frac{\partial T_g}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\lambda_g r^2 \frac{\partial T_g}{\partial r} \right) - c_{pg} \rho_g u_g \frac{\partial T_g}{\partial r} \quad (37)$$

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.

- Boundary condition for Eq. (37) at the drop surface ($r = r_d$) is similar to Eq. (27).
- Boundary condition for Eq. (37) at a far distance from the drop surface ($r \rightarrow \infty$):

$$\frac{\partial T_g}{\partial r} = 0 \quad (38)$$

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

$$\lambda_l \frac{\partial T_l}{\partial r} - \frac{\rho_{ls} u_s L_s}{W_v} = \lambda_g \frac{\partial T_g}{\partial r} \quad (39)$$

- Ideal gas equation of state (18) for the gas phase.
- Constant pressure condition:

$$p = p_0 \quad (40)$$

where p_0 is taken constant throughout the entire vaporization process.

Equations (22)–(40) were solved numerically with continuous monitoring of material and energy balance between liquid and gas phases. Detailed description of the numerical procedure is given in [7, 8]. All the results discussed below are obtained with the maximal allowable mass misbalance of 0.1%. To validate the detailed model, multiple comparisons have been made with available experimental data (see [7–9]). It was shown that the detailed model provides good predictions for liquid drops evaporating at microgravity conditions. It is worth emphasizing that the detailed model presented above does not contain any fitting parameter.

Results

The new vaporization model was compared with the Dukowicz model [2] which is often used in commercial CFD codes and with the detailed model of previous section for ambient gas (air) pressures ranging from 1 to 40 bar, and for gas temperatures ranging from 400 to 1500 K. Drops of three primary reference hydrocarbon fuels were considered, namely, *n*-heptane, *n*-octane, and *n*-decane. Only some results for *n*-heptane drops are presented herein. The initial diameter and temperature of *n*-heptane drops were taken equal to 50 μm and 293 K, respectively. The correction factor β (see Eq. (15)) was not varied in the calculations and was taken equal to 1.0.

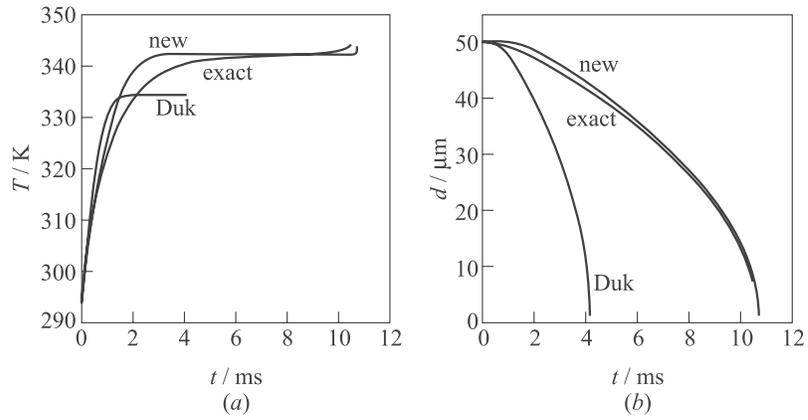


Figure 1 Vaporization of an *n*-heptane drop at $T_{g0} = 800$ K, $p = 1$ bar, and $T_{i0} = 293$ K: (a) mean temperature and (b) drop diameter histories

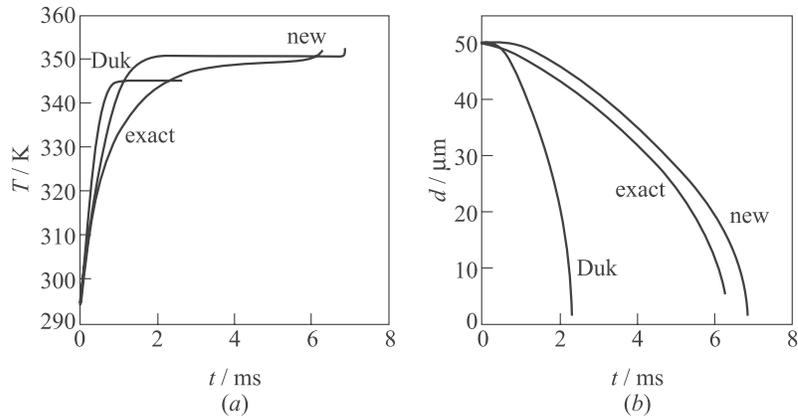


Figure 2 Vaporization of an *n*-heptane drop at $T_{g0} = 1200$ K, $p = 1$ bar, and $T_{i0} = 293$ K: (a) mean temperature and (b) drop diameter histories

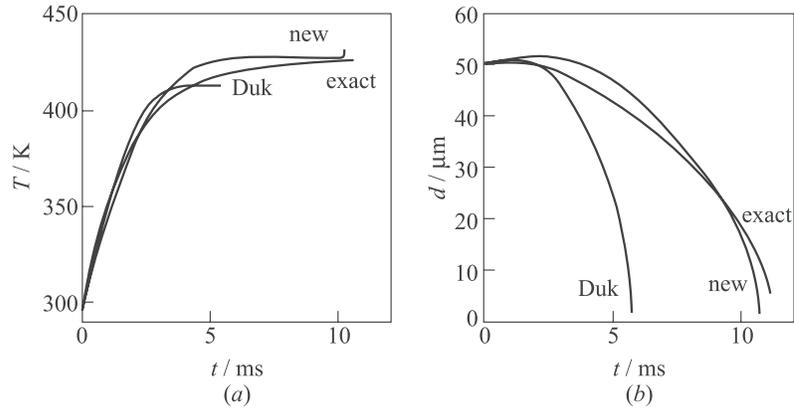


Figure 3 Vaporization of an *n*-heptane drop at $T_{g0} = 800$ K, $p = 10$ bar, and $T_{l0} = 293$ K: (a) mean temperature and (b) drop diameter histories

Figures 1 and 2 show the comparison between the Dukowicz model (curves denoted “Duk”) with the new model (curves denoted “new”) and detailed model (curves denoted “exact”) for a pressure of 1 bar and temperatures of 800 and 1200 K. It is seen from Figs. 1 and 2 that the new evaporation model predicts correctly the drop lifetime and the saturation (‘wet bulb’) temperature.

The Dukowicz model underestimates the ‘wet bulb’ temperature and drop lifetime. For example, at relatively low gas temperatures (see Fig. 1), the ‘wet bulb’ temperature in the Dukowicz model is by about 10 K less than in the exact solution. The drop lifetime predicted by the Dukowicz model can be up to 3–4 times less than that predicted by the detailed model, in particular, at high gas temperatures.

The correction of Eq. (15) coupled with the use of the mean drop temperature instead of various recommended ‘reference’ temperatures (for determining thermophysical properties of the gas) were found to play a decisive role in the improvement of model performance.

Figures 3 and 4 show a similar comparison for a pressure of 10 bar and temperatures of 800 and 1200 K. Again, the new model predicts correctly the drop lifetime and the ‘wet bulb’ temperature. At these

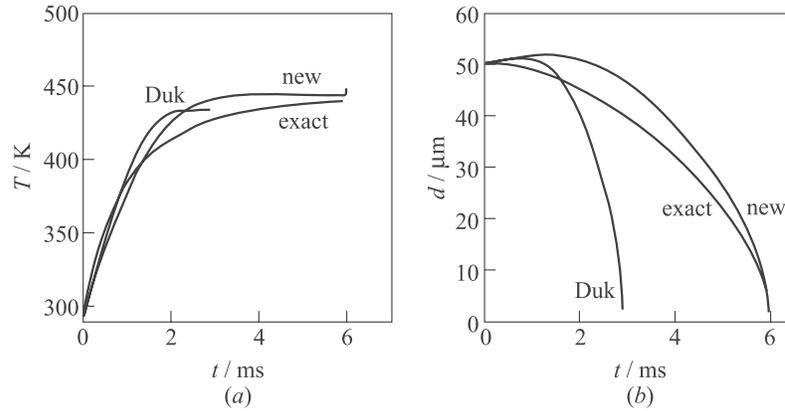


Figure 4 Vaporization of an *n*-heptane drop at $T_{g0} = 1200$ K, $p = 10$ bar, and $T_{i0} = 293$ K: (a) mean temperature and (b) drop diameter histories

conditions, the Dukowicz model underestimates the ‘wet bulb’ temperature and drop lifetime as well.

Concluding Remarks

Validation of the new drop vaporization model against the detailed model indicates that the former provides good predictions in terms of the ‘wet bulb’ temperature and drop lifetime within a wide range of gas temperature and pressure. In the cases when the new-model based solution is somewhat different from the exact solution, the drop lifetime is usually slightly underestimated or overestimated. Therefore, the correction coefficient β (see Eq. (15)) could be taken a bit smaller or 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 up to 3–4. For other liquid hydrocarbons, the new model also provides more realistic characteristic times of drop heating and vaporization.

Acknowledgments

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