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COMPARATIVE STUDY OF EQUILIBRIUM AND NONEQUILIBRIUM EVAPORATION MODELS FOR VAPORIZING DROPLET ARRAYS AT HIGH-PRESSURE

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Abstract. Combustion performances and emissions are mainly influenced by atomization, evaporation of fuel droplets and mixing of fuel and air. In particular, vaporization is often the rate-controlling process and is directly related to the specific fuel consumption of the engine and to pollutant formation. The present work focuses on two competing factors, which strongly influence the vaporization process, specifically: drop–drop interactions and high-pressure effects. Numerical predictions from equilibrium and nonequilibrium vaporization models are compared with the experimentally determined evaporation rate of droplet arrays at high-pressure conditions. The objective is to improve the predictive capabilities of spray models by introducing drop interaction effects in the modeling and by verifying which formulation of heat and mass transfer is able to model adequately their mutual interdependence at high-pressure.

Keywords: vaporization at high-pressure, drop–drop interaction, nonequilibrium evaporation models, light scattering

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1. Introduction

Liquid droplet vaporization in a high-pressure/temperature environment is of relevance to combustion science and technology, due to the need for developing high-pressure combustion devices such as liquid-propellant rockets, gas turbines and diesel engines. In order to calculate the evaporation rate of such droplets, equations are required to describe the mass, momentum and energy transfer between the droplet and its surroundings. Theoretical analysis is difficult because the equations must take into account drop–drop interaction and nonequilibrium effects. The latter have become increasingly important in modern propulsion systems due to the fact that vaporization occurs under conditions of large departure from equilibrium, measured in terms of temperature and/or pressure difference between the droplet and the carrier gas. The literature in this area is now extensive, addressing these problems at various levels of complexity (Imaoka and Sirignano, 2005; Leiroz and Rangel, 1995; Wong and Lin, 1992; Sangiovanni and Labowsky, 1982). However, as yet no conclusive evidence has been achieved due to a lack of reliable experimental data. This paucity of experimental data is attributable to the difficulties of performing controlled experiments on free droplets of micrometer size in a high pressure/high-temperature environment. As a first step in the solution of this challenging problem, the vaporization rate of droplet arrays of micrometer size under high-pressure conditions has been derived experimentally (Sun, 2006). From these measurements, an empirical correlation for the drag coefficient of interacting droplets was obtained. The latter is of relevance for the development of semiempirical models, aimed at providing an accurate and comprehensive prediction of the individual droplet drag, Nusselt and Sherwood numbers for the case of interacting vaporizing droplets. These global parameters together with the instantaneous droplet locations, size, and speed are important for less computer-intensive spray simulations.

Due to the complexity of spray calculations, the traditional modeling approach consists of specifying the governing equations for a single, isolated droplet including drag, convective heat, and mass transfer. The derived equations, corrected for drop–drop interaction effects, are then used for a subset of statistically representative droplets in various forms of computational spray models (Crowe et al., 1996). Concerning the vaporization of an isolated droplet, the classical approach uses an equilibrium evaporation model, which leads to the so-called $d^2$-law. Over the years, significant advances have been made to the classical method to include the effects of variable thermophysical properties (Yuen and Chen, 1976), transient liquid heating (Law and Sirignano, 1977) and gas-phase convection (Ranz and Marshall, 1952). Despite the noteworthy progress, the above-mentioned models cannot overcome the limitations inherent in
the approach based on equilibrium thermodynamics. Alternatively, more advanced evaporation models have been developed based on the Langmuir–Knudsen approach, where nonequilibrium effects can be relatively easily incorporated by specifying an appropriate molecular velocity distribution function within the Knudsen layer. Different formulations of nonequilibrium evaporation models have been proposed in literature (Bellan and Summerfield, 1978; Bellan and Hardstad, 1987; Young, 1993), characterized by a different degree of complexity in the choice of the molecular velocity distribution function.

This paper presents the preliminary results of an ongoing systematic evaluation of evaporation models capable of describing the vaporization of small hydrocarbon droplets in a high-temperature/pressure environment, as found in modern propulsion systems. The models considered here include three versions of the heat-mass transfer analogy models and two nonequilibrium models based on the Langmuir–Knudsen approach. The models are evaluated through comparison with experiments. First, isolated hydrocarbon droplets vaporizing in low and high-temperature environments are considered. Subsequently, the comparison is extended to droplet arrays vaporizing in high-pressure convective surroundings.

2. Model Description

The set of governing equations describing the temporal evolution of a single droplet embedded in a carrier gas is reported below. In order to facilitate model comparison, the system of equations is cast in a very general form and the model dependency is incorporated into the specific expressions employed for the momentum \( F \), mass \( \dot{M} \) and thermal energy \( \dot{Q} \) transfers between the droplet and the carrier gas:

\[
\begin{align*}
\frac{dx}{dt} &= \Delta v_d \\
-\frac{d\Delta v_d}{dt} &= \frac{F}{m_d} - g \\
4\pi r_d^2 \rho_d \frac{dr_d}{dt} &= -\dot{M} \\
m_d c_{vd} \frac{dT_d}{dt} &= \dot{Q} + \dot{M}L - Q_{AT}
\end{align*}
\]

(1)

where \( m_d \) is the droplet mass, \( c_{vd} \) the liquid heat capacity, \( \rho_d \) the liquid density, \( g \) the gravitational acceleration, \( L \) the latent heat of evaporation, and \( Q_{AT} \) represents any additional term used to incorporate nonuniform internal temperature effects (e.g., finite liquid thermal conductivity). These equations
represent a system of first-order ordinary differential equations for the droplet position \( x \), relative velocity \( \Delta v_{\text{rel}} \), droplet radius \( r_d \), and temperature \( T_d \). As starting conditions for the time integration, the initial droplet radius, position, temperature, and relative velocity are assigned. A real gas equation of state and generalized multiparameter estimation methods are employed for the determination of the thermophysical properties of the liquid droplet, vapor phase, and ambient gas (Sun, 2006).

2.1 MODELING OF TRANSFER RATES

The equations describing the quasisteady mass, momentum, and energy transfer between a single droplet and a carrier gas can be written as follows:

\[
\begin{align*}
\dot{M} &= 2\pi r_d D_m \rho_m S h_f M_f \\
\dot{Q} &= 2\pi r_d k_m (T_m - T_{\text{ref}}) N u_f Q_f \\
F &= \pi r_d^2 \rho_m \Delta v_{\text{rel}}^2 c_D
\end{align*}
\]

(2)

where \( D \) is the diffusion coefficient, \( k \) the thermal conductivity, \( c_D \) is the drag coefficient, \( N u \) and \( S h \), represent the Nusselt and Sherwood numbers, respectively and are empirically modified to account for convective effects. The subscript \( m \) refers to the reference state, which uses free stream conditions for the gas density and the so-called “1/3 rule” for all other properties. The factor \( f_M \) is directly related to the driving potential for mass transfer; \( f_Q \) represents, the correction to heat transfer due to the complementary role between heat and mass transfer. Their specific expressions can be found in Table 1, which identifies each evaporation model.

Five different models are selected for comparison. Among the three equilibrium formulations (termed MA1, MA2, and MA3, respectively), MA3 incorporates a correction for mass transfer accounting for higher departures from equilibrium. When the temperature difference between the drop and its surroundings is considerable, the rate of vaporization is a logarithmic function of the difference in vapor pressure at the drop surface and at infinite distance (Godsave, 1953). Additionally, models MA3 and MA1 also contain a correction for heat transfer (i.e., \( f_Q \neq 1 \)) derived on the basis of film theory (Spalding, 1953), which accounts for the cross-influence of mass transfer on heat transfer. As nonequilibrium formulations, two versions of Bellan’s Langmuir–Knudsen model are considered: LK1 simulates heat transfer inside the droplet using the infinite liquid conductivity hypothesis; LK2 includes finite liquid conductivity effects. Detailed descriptions of the models can be found in Bellan and Harstad (1987) and Miller et al. (1998) and hence, they are not repeated here.
TABLE 1. Expressions for the evaporation corrections $f_Q$, internal temperature gradient $Q_{\Delta T}$ and mass transfer potential $f_M$ from various models

<table>
<thead>
<tr>
<th>Model Name</th>
<th>$f_M$</th>
<th>$f_Q$</th>
<th>$Q_{\Delta T}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MA1 Mass analogy I</td>
<td>$B_M$</td>
<td>$\ln (1 + B_M)/B_M$</td>
<td>0</td>
</tr>
<tr>
<td>MA2 Mass analogy II</td>
<td>$B_M$</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>MA3 Mass analogy III</td>
<td>$\ln (1 + B_M)$</td>
<td>$\ln (1 + B_M)/B_M$</td>
<td>0</td>
</tr>
<tr>
<td>LK1 Langmuir–Knudsen</td>
<td>$\ln (1 + B_{M,neq})$</td>
<td>$G$</td>
<td>0</td>
</tr>
<tr>
<td>LK2 Langmuir–Knudsen</td>
<td>$\ln (1 + B_{M,neq})$</td>
<td>$G$</td>
<td>$(2\rho \delta/3 \tau_d Pr)(T_d - T_\infty)$</td>
</tr>
</tbody>
</table>

Nomenclature is as follows: $Y_{vr}$ is the vapor mass fraction at the droplet surface (the subscript $\infty$ refers to free steam conditions), $\theta_1$ is the ratio of gas heat capacity to that of the liquid phase $\theta_1 = c_{pg}/c_{vd}$, $Pr$ is the gas phase Prandtl number, $\tau_d$ is defined as $\tau_d = \rho_d D_d/18 \mu_s$, the subscripts $dr$ and $di$ refer to conditions at the droplet surface and inside, respectively. The nonequilibrium Spalding transfer numbers for mass ($B_{M,eq}$) and energy ($B_T$) are defined as

$$B_{M,(n)eq} = \frac{Y_{vr,(n)eq} - Y_{vr,eq}}{1 - Y_{vr,(n)eq}}, \quad B_T = \frac{c_{pm}(T_v - T_{dr})}{L}$$

where $L$ is the latent heat of vaporization. For the calculation of the parameters ($Y_{vr,eq}$, $Y_{vr,neq}$, $B_{M,eq}$, $B_{M,neq}$) and for the definition of the function $G$, the reader is referred to the work of Miller et al. (1998). Here, we simply recall that the function $G$ provides an analytical expression for heat transfer derived from the quasisteady solution of the gas field and contains explicitly the dependency on mass transfer. Essentially, this implies that for models LK1 and LK2 it is not necessary to employ empirical correlations to simulate the cross-influence between heat and mass transfer. However, the same consideration does not hold for the mass analogy models, where empirical correlations are required for the Nusselt and Sherwood numbers to reintroduce the mutual interdependency between heat and mass transfer into the modeling. For the present work, the Renksizbulut and Yuen (1983) correlations have been used

$$Nu = (2 + 0.57 Re_m^{1/2} Pr_f^{1/3})(1 + B_T)^{-0.7}$$

$$Sh = (2 + 0.87 Re_m^{1/2} Sc_f^{1/3})(1 + B_M)^{-0.7}$$

$$c_D = c_D^{en}(Re_m)(1 + B_T)^{-0.2}$$

where $Re$ is the Reynolds number ($Re = 2 \rho_v r_d v_d/\mu_v$), $Sc$ the Schmidt number ($Sc_f = \mu_f/\rho_f D_f$) and $Pr$ the Prandtl ($Pr_f = c_{pf} \mu_f/\kappa_f$). The drag coefficient of an isolated droplet is estimated using the correlation proposed by Virepinte et al. (1999). Note that, for models LK1 and LK2, the factor $(1 + B)^d$ in Eq. (4) is
retained only in the correlation for the drag coefficient, as the two models were initially developed for droplets evaporating in a stagnant environment and thus do not take into account the influence of heat transfer on momentum transfer.

Interaction effects are modeled by means of empirical correlations, expressing the reduction of mass transfer and drag coefficient in terms of the nondimensional interdroplet distance \((\Delta s/D_0)\). For the mass transfer, the correlation proposed by Atthisit et al. (2005) is employed:

\[
S_{h_{\text{prx}}} = S_h \left[ 1 - 0.57 \left( \frac{1 - e^{-0.13(\Delta s/D_0)^{-6}y}}{1 + e^{-0.13(\Delta s/D_0)^{-6}y}} \right) \right]
\]  

The latter is valid for \(2 < \Delta s/D_0 < 16\) and \(12 < Re < 25\). For the drag coefficient, instead, the correlation proposed by these authors is used. For a discussion on its derivation and accuracy, the reader is referred to Sun (2006)

\[
c_{D_{\text{prx}}} = c_{D_{\text{ev}}} \left[ 1 - a \exp(-b \frac{\Delta s}{D}) \right]
\]

where

\[
a = -0.9139 + 0.2955 \exp(-0.0244Re) \\
b = -0.0302 - 0.0634 \exp(-0.0132Re)
\]

3. Results and Discussion

The predictive capabilities of the different models are best evaluated through comparison with droplet vaporization experiments occurring in high-temperature/pressure convective environments, as those are more representative of the conditions normally encountered in modern propulsion systems. In an attempt to evaluate separately the accuracy of the models in capturing correctly both nonequilibrium and interaction effects, isolated droplet experiments are considered first followed by monodisperse droplet streams. Although the extent of experimental data is too limited to draw definite conclusions on model quality, it was possible to identify some specific trends.

3.1 ISOLATED DROPLET EXPERIMENTS

Figure 1a shows the temporal evolution of the relative surface area for a single water droplet \((D_0 = 1.1\) mm and \(T_{d,0} = 282\) K) evaporating in stagnant air at \(T_x = 298\) K. As can be immediately seen, all models predict identical evaporation histories and agree with the experiments. The temperature evolutions are also
basically identical for all models and approximately equal to the wet-bulb temperature, predicted by Miller’s formula (1998). As expected, for a small departure from equilibrium, all mass analogy models perform rather well. This result contradicts those of Miller et al. (1998), who still observed some slight differences in the temperature evolutions when employing the Ranz and Marshall (1952) correlation. In the present work, however, Renksizbulut and Yuen’s (1983) correlation is used, where the \( Nu \) and \( Sh \) numbers are nonlinear functions of the respective transfer numbers. This indicates that the latter is more capable of capturing the mutual interdependency between heat and mass transfer for low evaporation rates.

![Figure 1](image1)

Figure 1. Numerical predictions of the nondimensional droplet surface area compared to the experimental results from (a) Ranz and Marshall (1952). Initial conditions: \( T_s = 298 \, \text{K}, \, T_{db} = 282 \, \text{K}, \, D_0 = 1.1 \, \text{mm} \) and \( Re_d = 0 \); (b) Wong and Lin (1992). Initial conditions: \( T_s = 1000 \, \text{K}, \, T_{db} = 315 \, \text{K}, \, D_0 = 2.0 \, \text{mm} \) and \( Re_d = 17 \)
Variations among the model predictions start to appear as soon as the evaporation process occurs under conditions of high departure from equilibrium as in the experiments by Wong and Lin (1992). Their experiments consisted of a decane droplet with initial size $D_0 = 2.0$ mm and temperature $T_{d,0} = 315$ K evaporating in a convective airstream at $T_f = 1,000$ K. Figure 1b clearly reveals that in the initial phase of the vaporization process, corresponding to the heat up transient stage, the $d^2$-law is invalid. The results shown in Figure 1b suggest that the droplet size evolution is best modeled using either of the two nonequilibrium models. However, the mass analogy models clearly overestimate the droplet size. This is due to the fact that the droplet temperature is largely underestimated. The heat transfer reduction through the factor $(1 + B_M)^{-0.7}$ in Eq. (4) provides a relatively strong contribution, thus resulting in an underestimation of the droplet temperature. In model MA1 and MA2, the size prediction is somewhat improved by the stronger mass potential $B_M$ (when compared to $\ln (1 + B_M)$ of model MA3), which compensates somewhat for the reduced heat transfer, thus resulting in a faster evaporation rate.

3.2 INTERACTING DROPLET EXPERIMENTS

As a final verification, the numerical predictions from the various models are compared with our own experimental results (Sun, 2006). The objective is twofold. First, we intend to determine the accuracy and range of validity of each model with respect to high pressure effects. Second, we want to verify whether the proposed empirical correlations for $Sh^{pr}$ and $c_D^{pr}$ are indeed capable of simulating proximity effects among the droplets correctly. The results can be summarized as follows. Except for model MA3, the numerical results agree fairly well with the experiments as the chamber pressure is raised from 5 to 40 bar. For example, Figure 2 shows the temporal evolution of the nondimensional droplet surface area for two different chamber pressures. At low pressure, the larger deviations observed for model MA3 are due to the concomitant effect of the factors $f_M = \ln (1 + B_M)$ and $f_Q = \ln (1 + B_M)/B_M$ which results in a higher quenching of the mass transfer. For models MA2 and MA3, this effect is counterbalanced by the stronger mass potential $f_M = B_M$. At higher pressures (i.e., higher droplet Reynolds number), convective heat transfer becomes the dominant effect in controlling the rate of vaporization, thus overshadowing completely the role of the correction factor $f_Q$. The macroscopic result is no difference in the model predictions, as shown in Figure 2b. Both LK1 and LK2 perform very well at all chamber pressures without the need to employ any correction factors for the heat and mass transfer.

Figure 3 depicts the nondimensional droplet speed for the same experimental conditions shown in Figure 2. The results clearly show that its temporal
evolution is well captured by all models at all pressure levels. This indicates that the proposed correlation for the drag coefficient (Eq. (6)) together with the correction for the vaporizing case (Eq. (4)) is indeed able to model correctly the momentum transfer process in vaporizing arrays. The same conclusion holds for the proximity correction, proposed by Atthasit et al. (2005), for mass transfer, since it is demonstrated that the good performance of the correlation is independent from the specific vaporization model chosen.

![Figure 2](image_url)

*Figure 2.* Temporal evolution of the nondimensional droplet diameter squared: comparison between experimental results and numerical predictions for different chamber pressure (a) $P_c = 10$ bar and (b) $P_c = 40$ bar. Experimental conditions: $D_0 = 88 \mu m$ $T_0 = T_{10} = 315 K$, $\Delta x/D_0 = 3.2$, and $36 < Re_{D_0} < 236$
Figure 3. Temporal evolution of the nondimensional droplet speed: comparison between experimental results and numerical predictions for different chamber pressure (a) $P_f = 10$ bar and (b) $P_f = 40$ bar. Experimental conditions: $D_0 = 88$ µm $T_w = T_{d0} = 315$ K, $\Delta t/D_0 = 3.2$, and $36 < Re_{d0} < 236$.

References


Comparative Study of Evaporation Models


