

# Transport coefficients and life history of a vaporising liquid fuel droplet subject to retardation in a convective ambience

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## Abstract

A numerical model has been developed for the process of droplet evaporation in a convective surrounding of high temperature gas. The model is based on numerical solution of unsteady conservation equations of mass, momentum, energy and species for both the gas and liquid phase. The important feature of the work is the consideration of continuous variation in free stream velocity with respect to the drop. This has been made in consideration of varying slip velocity (the velocity of droplet relative to free stream gas) of a moving droplet in a gaseous medium in real situation. The temporal reduction in free stream velocity has been evaluated from the droplet drag determined by the pressure and velocity fields of the gas phase surrounding the droplet. The relationships of drag coefficient and Nusselt number with the controlling variables like Reynolds number and Prandtl number have been established in the case of varying free stream velocity relative to the droplet, and have been compared with the standard laws for constant slip velocity. Other important characteristics of vaporising droplet, like mass depletion history and temperature response, under the present situation, have been determined as a function of pertinent controlling parameters like initial Reynolds number of the droplet and the ratio of free stream to initial droplet temperature. © 1999 Elsevier Science Inc. All rights reserved.

**Keywords:** Convection; Diffusion; Free stream; Transport coefficient; Vaporization

## Notation

$a'$	radius of drop at any instant
$a$	non-dimensional $a'(a'/a_i^g)$
$B$	transfer number $[C_p^g(T_\infty' - T_s')/\Delta H_{vi}]$
$C$	mass fraction of liquid vapour
$C_p$	specific heat
$C_{sf}$	mass fraction of fuel vapour at surface
$D$	diffusivity of fuel vapour in ambience
$\Delta H_{vi}$	enthalpy of vaporisation of $k$ th species at the initial state
$Ku_i$	initial Kutataladeze number $[\Delta H_{vi}/C_{pi}^g T_i']$
$M$	molecular weight
$m$	mass of droplet
$Nu$	Nusselt number
$P'$	pressure
$P'_v$	vapour pressure
$P$	non-dimensional pressure $P'[(P' - P_\infty)/(\rho_i^g U_{\infty i}^2)]$
$Pe_i$	initial Peclet number $[(2U'_{\infty i} a'_i)/(a_i^g)]$
$Pr$	Prandtl number $[C_p^g/v_i^g]$
$Re_i$	initial Reynolds number $[(2U'_{\infty i} a'_i)/(v_i^g)]$
$r'$	radial coordinate
$r$	non-dimensional $r'(r'/a')$
$Sc$	Schmidt number $[v_i^g/D]$
$T'$	temperature

$T_i'$	initial drop temperature
$T_\infty'$	free stream temperature
$T_s'$	surface temperature
$T$	non-dimensional $T'(T'/T_i')$
$t'$	time
$t$	non-dimensional $t'[(t' \cdot \alpha_i^g)/a_i^2]$
$U'_\infty$	free stream velocity
$U_\infty$	non-dimensional $U'_\infty[U'_\infty/U'_{\infty i}]$
$\hat{V}'$	velocity vector
$\hat{V}$	non-dimensional $\hat{V}'[(\hat{V}' \cdot a_i^g)/\alpha_i^g]$
$V'_s$	velocity of stefan flow
$V_s$	non-dimensional $V'_s[V'_s/U'_{\infty i}]$
$\alpha$	thermal diffusivity
$\rho$	density
$\mu$	dynamic viscosity

## Superscript

g	gas phase
l	liquid phase
b	bulk value corresponding to drop

## Subscript

i	initial state
j	species identifier
m	mixture
r	radial component
$\theta$	azimuthal component
$\infty$	free stream boundary

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v vapour  
s drop surface

1. Introduction

Evaporation and combustion of liquid droplets and sprays are extensively used in a variety of devices ranging from simple fire sprinklers to complex propulsion systems associated with different process and power industries. The design of such devices or systems, namely, the combustion chamber, spray drier, cooling tower etc. depends primarily on the understanding of the physical interaction of an evaporating or burning spray with its surrounding medium. The evaporation rate of a spray is basically determined and controlled by the processes of heat, mass and momentum transport between the ambience and the liquid droplets constituting the spray.

The theory of fuel droplet vaporization and combustion, due to its inherent impact on the various industrial processes, has received a good deal of attention for its development by a large number of workers for several decades. A comprehensive documentation of the work in the field can be found in Marshall (1954), Chigier (1976), Clift et al. (1978), Law (1983), Faeth (1977, 1983, 1987) and Sirignano (1983, 1988). Fundamental information in this regard includes mainly the life time and the transport coefficients of an evaporating droplet in an unbounded gaseous medium under various conditions of free stream ambience. Most of the works, reported in literature, describe the vaporization process of a droplet for constant free stream velocity with respect to the droplet and furnish the empirical and numerical information in terms of the transport coefficients of droplet and its mass depletion history as a function of pertinent controlling variables. Special mention can be made in this regard, of the work of Marshall (1954) Agston et al., 1957 Yuen and Chen (1978), Renksizbulut and Yuen (1983a, b), Dash et al., 1991 and Dash and Som, 1991. All these works finally predict the typical  $d^2$  and  $d^{3/2}$  law for vaporization of a moving drop with a uniform slip velocity in spherico-symmetric case and convective situation, respectively.

In real situation, the slip velocity between the droplet and gas phase changes continuously due to droplet drag during the vaporization of a spray in a gaseous medium. However, a conclusive information regarding the influence of continuously varying slip velocity on the transport coefficients of a vaporising droplet is hardly found in literature. Therefore, an attempt has been made in the present work to develop a numerical model in predicting the transport coefficients of a vaporising droplet with a continuous variation in free stream velocity and to check the applicability of the existing laws, developed for constant free stream velocity, under the present situation. The model is based on the numerical solution of conservation equations (mass, momentum and energy) in droplet and gas phases. The change in free stream velocity with respect to droplet has been determined from its equation of motion on a Lagrangian frame, under the influence of a drag force calculated from the predicted velocity and pressure field of the gas phase.

2. Theoretical formulation

The physical problem describes the evaporation of a liquid droplet in a convective gaseous medium. The free stream temperature is higher than the initial temperature of the droplet. The free stream velocity of the gaseous medium (with respect to the droplet) is assumed to vary with time from an initial value. This variation in the free stream velocity is computed in consideration of the droplet drag.

The following assumptions have been made in the present model:

- The droplet maintains a perfect spherical shape at all times. This is justifiable because the droplet is small and hence the surface tension is high enough to prevent any distortion at the drop surface by the convective medium;
- The flow is laminar, incompressible and axi-symmetric. This is justified for the study at low Reynolds number usually encountered in droplet evaporation;
- Thermodynamic equilibrium exists at the gas liquid interface;
- The effects due to gravity and thermal radiation are neglected because of small droplet diameter and a relatively low temperature in the gas phase, respectively.

3. Governing equations

The conservation equations in both the phases are written in dimensionless form with respect to a spherical co-ordinate system (Fig. 1) with the origin at the center of the droplet. Overall mass continuity:

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 V_r) + \frac{1}{\sin \theta} \frac{1}{r} \frac{\partial}{\partial \theta} (V_\theta \sin \theta) = 0. \tag{1}$$

Momentum:  $r$ -direction:

$$\begin{aligned} \frac{\partial V_r}{\partial t} + \frac{Pe_i}{2} \frac{1}{a} \left[ \frac{\partial}{\partial r} (V_r^2) + \frac{1}{r} \frac{\partial}{\partial \theta} (V_r V_\theta) - \frac{V_\theta^2}{r} + \frac{2}{r} (V_r^2) + \frac{\cot \theta}{r} (V_r V_\theta) \right] \\ = - \frac{Pe_i}{2} \frac{1}{a} \frac{\rho_i^g}{\rho} \frac{\partial P}{\partial r} + \frac{Pe_i}{2} \frac{1}{a^2} \frac{\nu}{v_i^g} \left[ \frac{\partial^2 V_r}{\partial r^2} + \frac{2}{r} \frac{\partial V_r}{\partial r} + \frac{1}{r^2} \frac{\partial^2 V_r}{\partial \theta^2} \right. \\ \left. + \frac{\cot \theta}{r^2} \frac{\partial V_r}{\partial \theta} - \frac{2}{r^2} \frac{\partial V_\theta}{\partial \theta} - \frac{2}{r^2} (V_r) - \frac{2}{r^2} (\cot \theta V_\theta) \right]. \end{aligned} \tag{2}$$

$\theta$ -direction:

$$\begin{aligned} \frac{\partial V_\theta}{\partial t} + \frac{Pe_i}{2} \frac{1}{a} \left[ \frac{\partial}{\partial r} (V_r V_\theta) + \frac{1}{r} \frac{\partial}{\partial \theta} (V_\theta^2) + \frac{3}{r} (V_r V_\theta) + \frac{\cot \theta}{r} (V_\theta^2) \right] \\ = - \frac{Pe_i}{2} \frac{1}{a} \frac{\rho_i^g}{\rho} \frac{1}{r} \frac{\partial P}{\partial \theta} + \frac{Pe_i}{Re_i} \frac{1}{a^2} \frac{\nu}{v_i^g} \left[ \frac{\partial^2 V_\theta}{\partial r^2} + \frac{2}{r} \frac{\partial V_\theta}{\partial r} + \frac{1}{r^2} \frac{\partial^2 V_\theta}{\partial \theta^2} \right. \\ \left. + \frac{\cot \theta}{r^2} \frac{\partial V_\theta}{\partial \theta} + \frac{2}{r^2} \frac{\partial V_r}{\partial \theta} - \frac{1}{\sin^2 \theta} \frac{V_\theta}{r^2} \right]. \end{aligned} \tag{3}$$

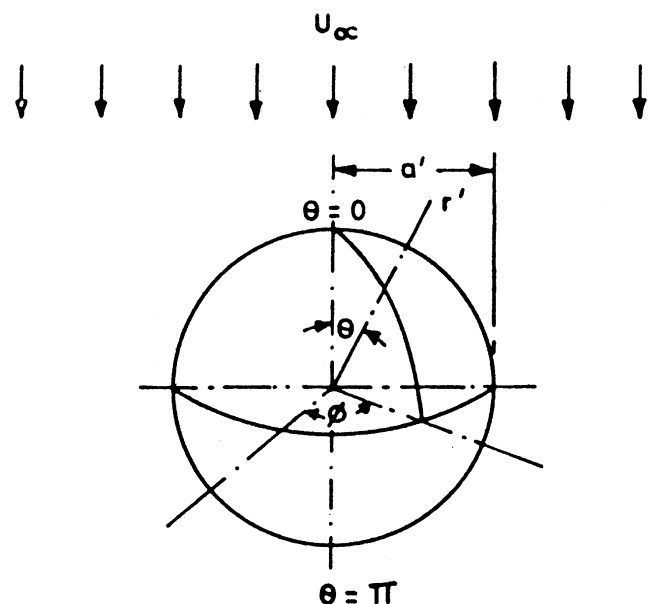


Fig. 1. System of co-ordinates and nomenclature used in the theoretical analysis.

Energy and species conservation: A general expression for the energy and species conservation equations in non-dimensional conservative form can be written as

$$\begin{aligned} \frac{\partial \phi}{\partial t} + \frac{\text{Pe}_i}{2} \frac{1}{a} \left[ \frac{\partial}{\partial r} (V_r \phi) + \frac{1}{r} \frac{\partial}{\partial \theta} (V_\theta \phi) + \frac{2}{r} (V_r \phi) + \frac{\cot \theta}{r} (V_\theta \phi) \right] \\ = \frac{G}{a^2} \left[ \frac{\partial^2 \phi}{\partial r^2} + \frac{2}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{1}{r^2} \cot \theta \frac{\partial \phi}{\partial \theta} \right]. \end{aligned} \quad (4)$$

The variable  $\phi$  and the parameter  $G$  (diffusivity) take specific values depending upon the cases as described later.

### 3.1. Initial and boundary conditions

Eqs. (1)–(4) are solved numerically for both the gas and the liquid phases with the aid of following initial and boundary conditions:

The initial conditions (at  $t=0$ ) are

for  $0 \leq r \leq 1$

$$V_r^l = V_\theta^l = P^l = 0, \quad T^l = 1 \quad (5)$$

and for  $r > 1$

$$V_r^g = -\cos \theta, \quad V_\theta^g = \sin \theta, \quad T^g = T_\infty, \quad C_f = 0, \quad P^g = 0. \quad (6)$$

Boundary conditions: At  $t \geq 0$ , the boundary conditions in the free stream ( $r \rightarrow \infty$ ) are:

for  $\theta = 0$  to  $\frac{\pi}{2}$

$$T^g = T_\infty, \quad C_f = 0, \quad V_r^g = -U_\infty \cos \theta, \quad V_\theta^g = U_\infty \sin \theta \quad (7)$$

for  $\theta = \frac{\pi}{2}$  to  $\pi$

$$\frac{\partial T^g}{\partial r} = \frac{\partial C_j}{\partial r} = \frac{\partial V_r^g}{\partial r} = \frac{\partial V_\theta^g}{\partial r} = 0. \quad (8)$$

At Interface ( $r=1$ ):

$$V_r^g = V_s, \quad V_r^l = 0, \quad (9)$$

$$V_\theta^g = V_\theta^l, \quad \tau_{r\theta}^g = \tau_{r\theta}^l, \quad (10)$$

$$T^g = T^l, \quad (11)$$

$$\frac{\partial T^g}{\partial r} = \frac{k^l}{k^g} \frac{\partial T^l}{\partial r} + \frac{1}{2} \text{Pe}_i \text{Ku}_i a \left( \frac{\Delta H_v}{\Delta H_v} \frac{C_{p_i}^g}{C_{p_i}^l} \frac{\alpha_i^g}{\alpha_i^l} \right) V_s. \quad (12)$$

At drop centre ( $r=0$ ):

$$\frac{\partial T^l}{\partial r} = 0. \quad (13)$$

Axi-symmetric conditions (at  $\theta = 0$  and  $\pi$ ):

$$V_\theta^g = V_\theta^l = 0, \quad (14)$$

$$\frac{\partial V_r^g}{\partial \theta} = \frac{\partial V_r^l}{\partial \theta} = \frac{\partial T^g}{\partial \theta} = \frac{\partial T^l}{\partial \theta} = \frac{\partial C_j}{\partial \theta} = 0. \quad (15)$$

Vapour mass fraction at droplet surface:

$$C_{s_f} = \frac{1}{1 + \left( \frac{M_a}{M_f} \right) \left( \frac{P_\infty}{P_s} - 1 \right)}. \quad (16)$$

Radial velocity at droplet surface ( $V_s$ ):

From the consideration of an impermeable interface to all the non-evaporating species, the radial velocity at the droplet surface,  $V_s$ , can be written as

$$V_s = \left( -2 \frac{\partial C_f}{\partial r} \Big|_{r=1} \right) / [a \text{Re}; \text{Sc} (1 - C_{s_f})]. \quad (17)$$

Depletion of droplet diameter:

In the context of spherical shape assumption, a uniform depletion rate of droplet diameter for all azimuthal angles is considered, and is given by

$$\frac{da}{dt} = -\frac{\rho_s}{\rho^l} \frac{\text{Pe}_i}{2} \bar{V}_s \quad (18)$$

where,  $\bar{V}_s$  is the surface averaged value of  $V_s$ .

Transport coefficients:

Nusselt number:

Instantaneous values of local and surface averaged Nusselt number are found from

$$\text{Nu}_\theta = \left( -2 \frac{\partial T^g}{\partial r} \Big|_{r=1} \right) / (T_\infty - T_s), \quad (19)$$

$$\text{Nu} = \frac{1}{2} \int_0^\pi \text{Nu}_\theta \sin \theta \, d\theta. \quad (20)$$

Drag coefficient:

The drag coefficient  $C_D$  is found from

$$C_D = F_D / (0.5 \rho_1^g U_\infty^2 \pi a^2). \quad (21)$$

The drag force  $F_D$ , experienced by the drop under the present situation, can be expressed as the sum of the three component forces contributed by pressure, friction and evaporation as

$$F_D = F_{D_p} + F_{D_f} + F_{D_E}, \quad (22)$$

where,

$$F_{D_p} = 2\pi a^2 \int_0^\pi P'_\theta \cos \theta \sin \theta \, d\theta, \quad (23)$$

$$F_{D_f} = 2\pi a^2 \int_0^\pi (\sigma'_{rr} \cos \theta - \sigma'_{r\theta} \sin \theta) |_{r=a} \sin \theta \, d\theta, \quad (24)$$

and,

$$F_{D_E} = 2\pi a^2 \int_0^\pi (V'_\theta \sin \theta - V'_s \cos \theta) |_{r=a} V'_s \sin \theta \, d\theta. \quad (25)$$

Reduction of free stream velocity  $U_\infty$  with time:

Since the coordinate axes are fixed to the droplet centre, the free stream velocity in the present analysis represents the slip velocity between the droplet and gas phase in a real situation, where the droplets at high velocity are injected into a continuous gas phase with a constant free stream velocity. A continuous change in slip velocity takes place, in this situation, due to retardation of the moving droplet because of the drag force exerted by the gas phase. Following this line of thought, the reduction in free stream velocity  $U_\infty$  with time  $t$  in the present case, has been determined in consideration of the droplet drag in the following way:

$$\frac{dU_\infty}{dt} = -\frac{a^2}{2} \frac{1}{\alpha_i^g} \frac{F_D}{U_\infty m}. \quad (26)$$

Eq. (26) is solved explicitly by fourth order Runge–Kutta method with the initial condition  $U_\infty = 1.0$  at  $t=0$ .

## 4. Method of solution

Eqs. (1)–(4) were discretised and solved simultaneously following an explicit finite difference technique. For the solutions of equations in the gas phase, a co-ordinate transformation ( $r = e^r$ ) was made in the radial direction to get denser

mesh near the droplet surface as suggested by Woo and Hamielec (1971). The variables were defined in the solution domain following a staggered grid arrangement. The convective and diffusive terms were discretised by hybrid and central differencing schemes, respectively. The solution of momentum Eqs. (2) and (3) along with the mass continuity Eq. (1) was carried out by a computing technique developed after the Hirt and Cook (1972) formulation of the original MAC (Marker and Cell) method due to Harlow and Welch (1965). A time dependant solution was obtained by advancing the flow field variables through a sequence of short time steps. The time steps were determined comparing the Courant–Friedrichs–Lewy (CFL) condition and the restriction on grid Fourier number so that any numerical instability could be avoided.

In the gas phase, mesh size ( $\Delta z \times \Delta \theta$ ) of  $0.05 \times 6^\circ$  with  $z_\infty = 4$  (corresponding to a non-dimensional  $r = 54.6$ ) was adopted as suggested by Sayegh and Gauvin (1979), and also confirmed by the work of Ghosal (1993) for grid sensitivity. In the liquid phase, a uniform sized grid with ( $\Delta r \times \Delta \theta$ ) of  $0.05 \times 6^\circ$  was taken.

The instantaneous drop radius was determined from Eq. (18) by the modified Euler's method with the initial condition as  $a = 1$  at  $t = 0$ . In the computational scheme, the droplet lifetime referred to the instant when approximately 95% of the mass had burnt out which corresponds to the value of  $a \cong 0.36$ . The computation was not carried out beyond this time.

The studies were made with air as the free stream ambience and *n*-hexane ( $C_6H_{14}$ ) as the fuel constituting the droplet. The initial droplet temperature  $T'_i$  and free stream temperature  $T'_\infty$  were taken to be 300 and 900 K, respectively. Gas phase was considered to be a mixture of ideal gases (air and fuel vapour) and its thermo-physical properties were assumed to be spatially constant but updated with time. The property values for gas phase were evaluated at the film condition with the help of Reid et al. (1977).

## 5. Results and discussion

### 5.1. Comparisons of transport coefficients predicted by the present model with the existing information in the literature in the case of constant free stream velocity

Fig. 2 shows the comparison of drag coefficient  $C_D$  predicted by the present numerical model with the standard drag correlation for a non-evaporating droplet from the literature (Clift et al., 1978). It is found that the computed values of  $C_D$  agrees fairly well (with a deviation from 3% to 15%) with the standard drag curve without a transfer number ( $B$ ) correction. In fact the transfer number correction for evaporation is not needed provided the Reynolds number is defined on the basis of mixture viscosity  $\mu^s$  (with 1/3rd rule) and free stream density  $\rho_\infty$ . This was explained earlier by Yuen and Chen (1976) and Dash (1989) that the values of  $C_D$  for both evaporating and non-evaporating droplets remain almost the same due to counter weighing effects of marginal increase and decrease in  $C_{Dp}$  and  $C_{Df}$ , respectively. Moreover, the values of  $C_{DE}$  are less by one to two orders of magnitude as compared to  $C_{Dp}$  and  $C_{Df}$ . All properties defining Reynolds number used in standard drag correlation are referred to those at film conditions except for density which is the free stream density ( $\rho_\infty^s$ ).

Fig. 3 shows the comparison of Nusselt number predicted by the present model with the widely referred empirical equations due to Renksizbulut and Yuen (1983b) and Ranz and Marshall (1952). There is an excellent agreement of the predicted values from the present model with those of Renksizbulut and Yuen (1983b), while a relatively poor agree-

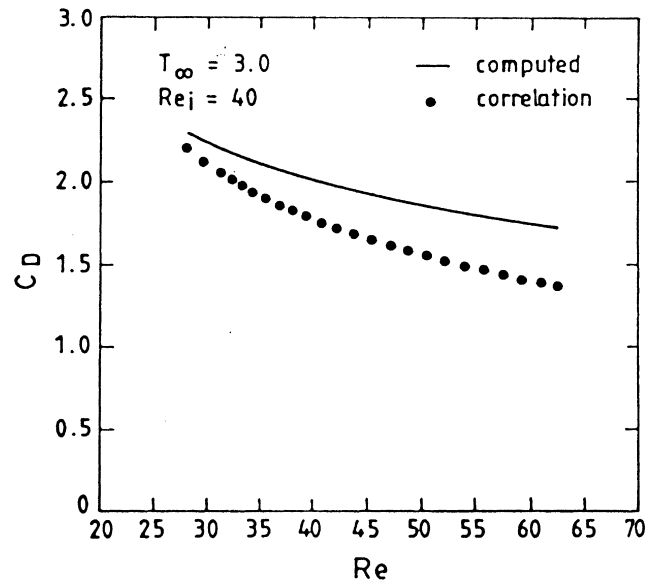


Fig. 2. Comparison of  $C_D$ , in case of an evaporating droplet with constant slip velocity, predicted by the present model with standard correlation from the literature.

ment (a deviation from 10% to 20%) is found with the empirical values reported by Ranz and Marshall (1952). This may be attributed to the fact that any empirical formula for  $Nu$  depends upon the range of transfer number  $B$  covered in the experiments which indicates the extent of evaporation, and the way [i.e. whether film condition (1/2 rule) or 1/3 rule] the average properties of the gas phase is defined. The steep part in the computed line of  $Nu$  (near the value of  $Re^{1/2}Pr^{1/3} = 12$ ) corresponds to the initial transience in droplet heating typical to a process of droplet evaporation. However, the part cannot be compared with the experimental data generated from steady state empirical laws of heat transfer.

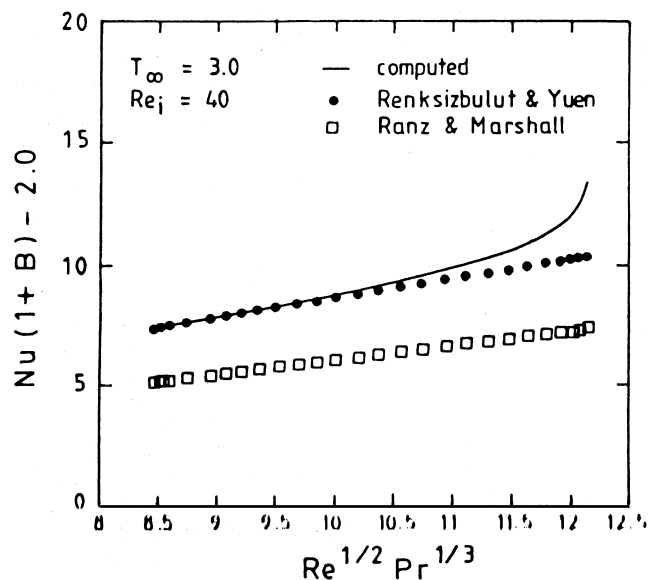


Fig. 3. Comparison of  $Nu$ , in case of an evaporating droplet with constant slip velocity, predicted by the present model with the standard empirical correlation from the literature.

5.2. Comparisons of transport coefficients for constant and continuously varying free stream velocity

The values of drag coefficient  $C_D$  have been computed from the present model for the situations with constant free stream velocity and with continuously varying free stream velocity (due to droplet drag). The functional relationship of  $C_D$  with instantaneous  $Re$  for both the cases are shown in Fig. 4. It is observed from the figure that there is virtually no difference between the relationship of  $C_D$  with  $Re$  in two cases. This concludes that the continuous variation in slip velocity (i.e. the velocity of free stream with respect to drop) due to droplet drag has practically no influence on the typical  $C_D$  vs.  $Re$  relationship with constant slip velocity. In other words, one can use the  $C_D$  vs.  $Re$  relation for a constant slip velocity, already available in the literature, to predict the value of  $C_D$  in case of a retarding or accelerating drop in practice by substituting the instantaneous  $Re$  in the drag law ( $C_D$  vs.  $Re$  relation) of constant slip velocity.

The comparison of Nusselt number predicted from the present model for the cases with uniform free stream velocity and continuously varying free stream velocity, as shown in Fig. 5, depicts the same picture as obtained in the case of drag coefficient, that there is no need of computing  $Nu$  in case of varying free stream velocity; rather the law of heat transfer, i.e.  $Nu$  vs.  $Re$  and  $Pr$  relation for a constant free stream velocity would be accurate enough for its use in case of a varying slip velocity of a moving drop in practice.

5.3. Comparison of life histories for vaporising droplet under constant and continuously varying slip velocities

It is observed from Fig. 6 that, a continuous change in free stream velocity has no influence on the transient response of droplet surface temperature  $T_s$ . It is found that for  $Re_i = 40$  and  $T_\infty = 3.0$ , the free stream velocity in the present model, representing the velocity slip in the case of a moving droplet, is reduced to 19% of its initial value as computed from Eq. (26) due to droplet drag, when the droplet diameter attains 36% of

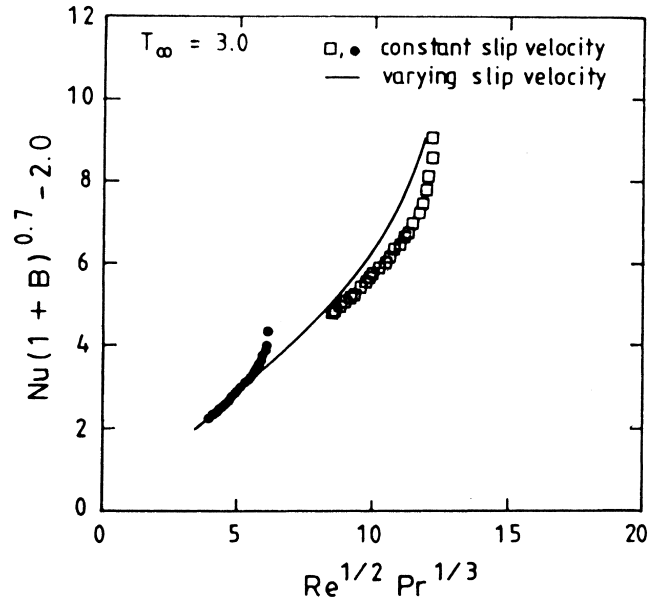


Fig. 5. Variation of  $Nu$  with  $Re$  and  $Pr$  of an evaporating drop in the case of constant and varying slip velocity.

its initial value corresponding to a mass depletion of 95%. It is obvious that for the same  $Re_i$  and  $T_\infty$  the lifetime of a droplet with continuous reduction in slip velocity is more as compared to that with constant slip velocity (Fig. 6), even if the calculations in both the cases are based on the same laws of transport processes. This is because, at any instant, the Reynolds number of a decelerated drop is lower (due to a decrease in both its diameter and slip velocity) and results in a relatively lower rate of mass transfer as compared to that of a drop with uniform slip velocity. However, in both the cases a linear variation in  $a^{3/2}$  with time  $t$  is observed.

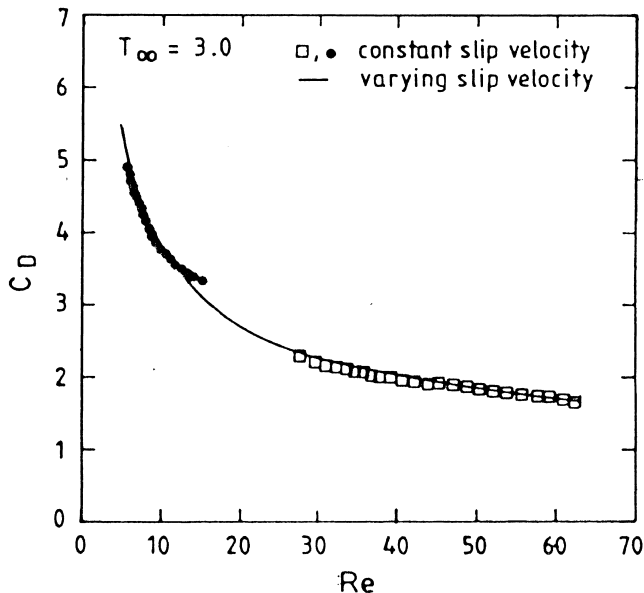


Fig. 4. Variation of  $C_D$  with  $Re$  of an evaporating drop in the case of both constant and varying slip velocity.

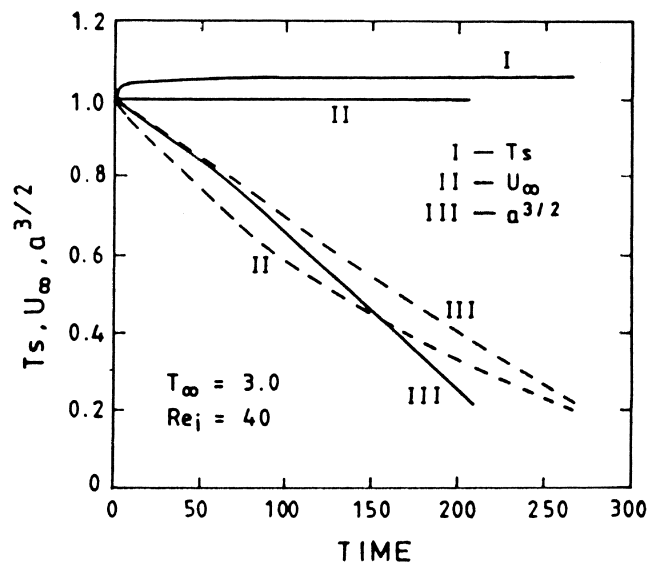


Fig. 6. Temporal histories of droplet size and surface temperature under constant and varying slip velocity (— constant slip velocity, - - - varying slip velocity).

## 6. Conclusions

A numerical model of droplet vaporization in a convective ambience with continuously varying free stream velocity determined from droplet drag has been developed to predict the transport coefficients of a vaporizing droplet. It has been recognised that a continuous change in free stream velocity with respect to the droplet, depicting acceleration or retardation of a moving droplet in a gas phase, has negligible influence on the standard drag and heat transfer laws (i.e. the relationships of drag coefficient with Reynolds number and that of Nusselt number with Reynolds number and Prandtl number) in case of constant free stream velocity with respect to the droplet.

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