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Mass transfer to an accelerating multidrop system

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1. INTRODUCTION

A DETAILED analysis of the dynamics and transport mechanisms of interacting drops is important for the basic understanding of (dense) spray processes and for a variety of absorption, drying, cooling and combustion systems. In *dense* sprays, drops are so closely spaced that they interact with each other and thereby modify the local ambient conditions including drop dynamics, fluid properties and heat/mass transfer rates. Of particular interest here are the momentum and mass transfer with chemical reaction of accelerating and interacting drops on a one-dimensional trajectory at moderate to high Reynolds numbers, i.e. the range of $50 < Re < 400$. The lower limit allows the use of boundary-layer type postulates and the upper bound is given by the sphericity assumption of liquid drops.

Recent reviews of theoretical and experimental modeling results for predominantly combustion sprays have been contributed by Sirignano [1], Faeth [2], Law [3] and Bracco [4]. For example, Tal and Sirignano [5] and Tal *et al.* [6] discussed the fluid mechanics and heat transfer for sphere arrays using their cylindrical cell model which is an improvement over the classical spherical cell model due to Happel [7]. The drop spacing is given by the 'voidage' of the sphere assemblage where each sphere is in a fixed position surrounded by a rectangular cell. Since the voidage is directly related to the inter-drop distance, the lumped parameter effects of different geometric array parameters can be evaluated. However, the interaction dynamics of several individual drops and hence distributed parameter effects cannot be calculated. Bracco [4] reviewed mathematical models and supportive experimental data for engine sprays considering droplet break up, dense spray and dilute spray regions. Bracco and co-workers used the discrete droplet model (DDM) with appropriate probability density functions to study for dense sprays the effect of void fraction on interphase transport rates (which was found to be weak) and the effect of drop collisions on drop size increase (which was found to be significant). These modeling approaches result in average system parameters, i.e. no details of the velocity/pressure and concentration fields around or within individual, interacting drops can be extracted. On the other hand, statistical models are computationally very cost-effective in estimating integral properties of entire spray regions.

In this paper we concentrate on several spherical monodispersed drops which interact while falling through a polluted environment. The work is based on a series of previously published papers [8–10] which concentrated on absorption of a trace gas (e.g. sulfur dioxide) by gravity sprays.

2. MATHEMATICAL FORMULATION

A mathematical model is developed to simulate the mass transfer characteristics of a multidrop system, falling vertically on a one-dimensional trajectory. Based on a previous analysis [11], five drops are being considered to calculate the drop dynamics, followed by a three-drop analysis of mass transfer, i.e. trace gas absorption with liquid phase chemical reaction.

2.1. *Drop dynamics*

The following analysis is based on the assumptions that:

(a) monosized drops are released with the same initial velocity at a regular time interval, i.e. at constant frequency; possible drop coalescence is presently not considered;

(b) the acceleration/deceleration phase of the first three drops is of major interest;

(c) a drop inbetween neighboring drops will experience both a 'front sphere effect' and a 'back sphere effect' as has been experimentally observed [15, 16]; the average of these effects is experienced by the center drop;

(d) in focusing basically on the first three drops, the development of the air entrainment corridor [8] is not treated separately but included in a modified approach velocity and the wake velocity field for mass transfer.

The governing equation for the motion of the ith drop is Newton's second law which can be written as

$$\frac{dv_i}{dt} = g\left(1 - \frac{\rho_a}{\rho_p}\right) - \frac{3}{8}\frac{C_{D,i}}{a}\frac{\rho_a}{\rho_p}v_i^2; \quad i = 1, \ldots, 5. \tag{1}$$

At any time, the dimensionless drop distance can be calculated from

$$d_{j,j+1} = (x_j - x_{j+1})/a; \quad j = 1, \ldots, 4 \tag{2}$$

where

$$dx_i/dt = v_i. \tag{3}$$

Based on the semi-empirical expressions given by Rowe and Henwood [12], the following equations are proposed for the

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NOMENCLATURE

a	radius of the drops [L]
b	half maximum radius (cf. ref. [15] or ref. [16])
c	concentration [ML^{-3}]
c_1, c_2	coefficients [L]
C_D	drag coefficient
d_{ij}	dimensionless interdrop distance ($d_{ij} = d_{ij}^*/a$)
f	frequency [T^{-1}]
g	acceleration due to gravity [LT^{-2}]
Re	Reynolds number ($Re = u_0 a/\nu_a$)
r, z	control volume coordinates
t	time [T]
t_0	elapsed time (d_{ij}^*/u_0) [T]
u_0	average of the velocities of drops 'i' and 'j' [LT^{-1}]
v	velocity [LT^{-1}]
x	fall distance [L].

Greek symbols

δ	control volume dimension [L]
ν	kinematic viscosity [L^2T^{-1}]
ρ	density
τ	non-dimensional time.

Subscripts

a	air
D	drag
g	gas phase
i	ith drop
j	drop index
k	drop index
0	initial
p	particle, drop
r	radial direction
s	single sphere
z	axial direction
∞	ambient.

Superscript

*	dimensional quantity.

drag coefficients of the drops

$$\frac{C_{D,1}}{C_{D,s}} = 1 + \frac{c_1}{2d_{12}} \tag{4}$$

$$\frac{C_{D,k}}{C_{D,s}} = \frac{1}{2}\left[\left(1 + \frac{c_1}{2d_{k,k+1}}\right) + \left(1 - \frac{c_2}{2d_{k-1,k}}\right)\right]; \quad k = 2,3,4 \tag{5}$$

and

$$C_{D,5}/C_{D,s} = 1.0 \tag{6}$$

where the standard drag correlation for single drops [14]

$$C_{D,s} = \frac{24}{Re} + \frac{6.0}{1+\sqrt{Re}} + 0.4. \tag{7}$$

The initial condition for equation (1) is

$$x_i = 0 \quad \text{and} \quad v_i = v_0 \quad \text{at} \quad t = t_i \quad \text{where} \quad t_i = (i-1)/f. \tag{8}$$

Computer experiments showed [11], that the free parameters c_1 and c_2 are rather insensitive to changes in multidrop system characteristics and hence the measured values [12], $c_1 = 0.151$ and $c_2 = 0.846$ are being used. In addition, it was observed and experimentally verified (cf. Section 4) that our postulates, i.e. equations (5) and (6) are correct. For the fifth drop, a single sphere drag coefficient can be used. Equation (7) is appropriate for the last drop as long as the drop dynamics of the first three drops are not affected. Indeed, the drop behavior of the first three drops was identical for both a five- and a seven-drop system [11].

2.2. *Mass transfer*

In order to obtain the local ambient conditions experienced by a stream of drops, a 'wake mass transfer model' has been developed. This model gives the local conditions (e.g. reduced trace gas concentration) as a function of interdrop distance and the local Reynolds number. The wake transfer model combined with the drop dynamics (cf. Section 2.1) and the detailed single drop mass transfer model (cf. Fig. 1(b) and ref. [12]) constitutes a comprehensive and flexible computer simulation model for the analysis and design of simple multiple drop systems.

2.2.1. *Single drop mass transfer model.* The appropriate forms of the transient convection–diffusion mass transfer equation with chemical reaction has been solved for the coupled gaseous and liquid phase of a single, moving drop [9]. Ramachandran *et al.* [9] showed that the single drop analysis overpredicts absorption rates for a stream of closely spaced drops. Thus, the interactive drop dynamics effects (cf. Section 2.1.) and the 'wake effect' of a reduced trace gas concentration have to be incorporated in order to obtain accurate results for simple multidrop systems.

2.2.2. *Wake mass transfer model.* Consider two representative drops, i and j, a distance d_{ij}^* apart, moving through a control volume of radius $\delta_r^* = 2b^*$ and length $\delta_z^* = d_{i,i+1} - 2a$. As the leading drop, i, leaves the control volume, unsteady state mass transfer from the global ambient takes place during an interval t_0, the time which elapses while each of the two drops crosses the midpoint of the region (Fig. 1). At the end of the time t_0, the average concentration in the control volume is assumed to be the new local ambient concentration as 'seen' by the succeeding drop j. Hence, for the three-drop system considered in the present study, the model is used to calculate the local ambient concentrations for drops 2 and 3, whereas the leading drop, 1, experiences the global ambient concentration. For the velocity field, needed in the mass transfer equation, the empirical wake velocity profiles of Hama and Peterson [15] are used. Hama and Peterson [15] developed expressions for v_r and v_z for

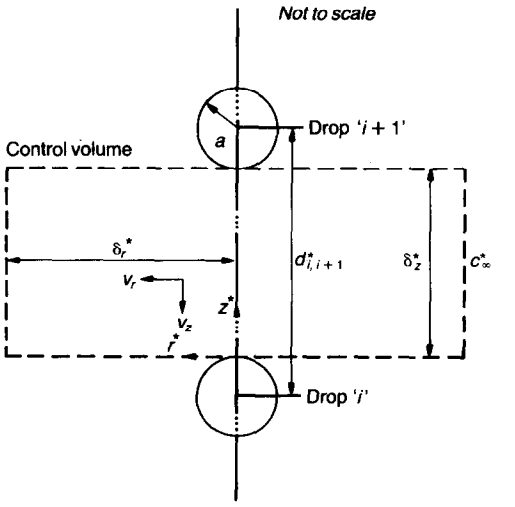

FIG. 1. Control volume for wake mass transfer calculations.

an axisymmetric laminar wake behind a slender body of revolution, based on experimental and theoretical analyses. Though the above wake velocity field does not account for separation effects, the fact that it is valid for the near wake region of a slender body of revolution suggested the use of these velocity profiles for wake mass transfer calculations. Further details of the wake mass transfer analysis can be found in a separate paper [16].

3. NUMERICAL SOLUTION

The drop dynamics model (Section 2.1), the detailed single drop mass transfer model (Section 2.2.1 and ref. [9]) and the wake mass transfer model (Section 2.2.2 and ref. [16]) are combined into a comprehensive model with which mass transfer characteristics of a system of three drops falling one behind the other are simulated. It can be summarized as follows:

(1) The 'drop dynamics' submodel is called to calculate, for a specific time step ($t_i \rightarrow t_f$), the velocities and the positions of the drops; from the positions, one can compute the interdrop distances, d^*_{12} and d^*_{23}.

(2) With each interdrop distance the wake mass transfer submodel is called to estimate the average local ambient conditions, as seen by drops 2 and 3; it should be noted that the leading drop, 1, is assumed to experience the global ambient concentration.

(3) Finally, with the local ambient conditions for each of the drops the detailed single drop mass transfer model is called to calculate the amount of gas absorbed by each drop.

A modified user-oriented package DSS/2 (Differential System Simulator, version 2 [17]) has been used to perform all calculations [11]. The software package has been modified to include: (a) conjugated boundary value problems for multiple regions and (b) a faster iteration scheme since numerous compatibility conditions have to be fulfilled at the common boundaries. The accuracy of the numerical scheme has been successfully tested by comparing well-defined subsystems with experimental data sets [8–10]. Independence of the results from the mesh density was checked. Additional computational details can be found in ref. [11].

4. RESULTS AND DISCUSSION

As indicated in the previous section, mass transfer predictions for the subsystem 'accelerating single drop' compared very well with experimental data sets [9]. The drop dynamics (cf. Section 2.1) of the first three drops for a five- and a seven-drop system has been qualitatively verified via flow visualization in a telescopic reactor described by Lindjhem [18]. The comprehensive model has been compared with SO_2 absorption data measured by Lindjhem [18]. The initial and ambient conditions used are given in Fig. 2 which depicts the total amount of sulfur absorbed by the accelerating drop stream as a function of fall height. The solid lines are the values computed for the first, second and third drop. The amount absorbed by the second and third drop is also within the range of experimental uncertainty (i.e. $\pm 1\ \mu\text{mol}\,\text{l}^{-1}$). The actual trace gas concentrations 'seen' by the succeeding drops do not differ greatly from the global ambient concentration because the interdrop distances are large for the given release frequency. However, even at relatively low frequencies, $f < O(100)$, some interaction effects on the mass transfer rate can be detected. Figure 2 shows that the amount absorbed by the fluid drops exceeds that of the second drop because drop 3 is less influenced by the preceding drops. This is well documented in Fig. 3 which shows that the dimensionless interdrop distance, d_{12}, between the first two drops decreases and hence the trace gas removal effect of drop 1 on drop 2 becomes more pronounced with

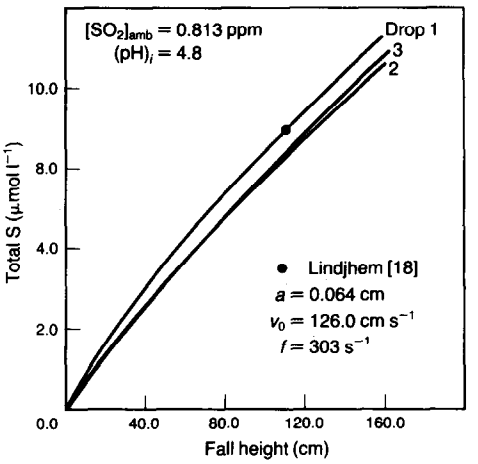

FIG. 2. Model comparison with experimental data [18].

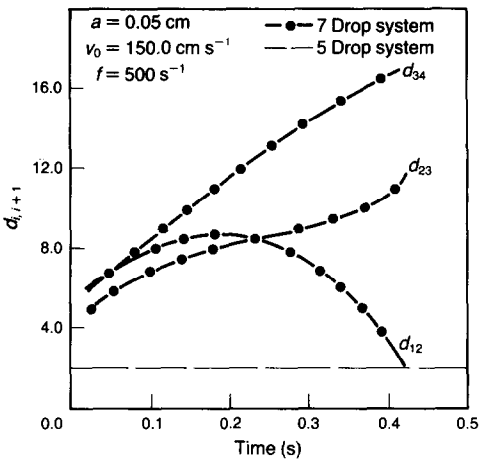

FIG. 3. Comparison of the drop dynamics of the first three drops for a five- and a seven-drop system.

time. The drop spacings between the third and second drop, d_{23}, and between drops 4 and 3 increase rapidly with time which implies that drop 3 is less affected by the interaction dynamics and drop 4 only negligibly so.

Additional computer experiments shows that the system parameters which strongly influence the drop dynamics and hence the mass transfer process of a multidrop system include drop diameter, frequency of drop release and initial velocity. In summary, the resistance to mass transfer is higher for larger drops so that the bigger drops absorb less. With an increase in frequency the interdrop distance decreases and hence the local ambient trace gas concentration as experienced by the succeeding drops is less, resulting in a reduction of the total amount of sulfur species absorbed. With an increase in initial velocity, the actual drop velocity and hence the Peclet number is higher at any time which is reflected in higher trace gas concentrations at a given exposure time. In addition, an increase in initial velocity results in larger interdrop distances which implies a higher local ambient concentration surrounding each drop within a stream of drops.

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Steady-state temperature distribution in a doubly connected, orthotropic region with heat generation

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INTRODUCTION

AS SHOWN in several recent papers [1–3] the Rayleigh–Schmidt approach is quite convenient when determining approximate analytical solutions to many important solid mechanics problems. The methodology has recently been applied in the case of heat conduction problems [4, 5] and it is extended herewith to the important practical situation of orthotropic regions which appears quite frequently in biomechanics, nuclear engineering, etc.

The title problem is solved by conformally transforming the given region in the z-plane onto an annulus in the ξ-plane. The transformed functional is approximately satisfied using a two-term solution and employing the Rayleigh–Schmidt criterion.

APPROXIMATE SOLUTION

The problem under study is governed by the orthotropic Poisson equation:

$$k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + q = 0 \tag{1a}$$

subjected to the boundary condition

$$T[L_i(x, y) = 0] = 0; \quad i = 1, 2 \tag{1b}$$

where $L_i(x, y) = 0$ is the functional relation which defines each boundary of the doubly connected domain.

In order to apply the Rayleigh–Schmidt formulation one expresses (1a) in terms of the equivalent functional

$$J[T] = \int\int_D \left[\frac{k_x}{2}\left(\frac{\partial T}{\partial x}\right)^2 + \frac{k_y}{2}\left(\frac{\partial T}{\partial y}\right)^2 - qT\right] dx\, dy \tag{2}$$

subjected to the condition (1b).

Let

$$z = x + yi = f(\xi); \quad \xi = re^{\theta i} \tag{3}$$

be the mapping function which conformally transforms the given domain onto an annulus in the ξ-plane.

Substituting (3) in (2) results in the transformed functional

$$J[T] = \frac{1}{4}\int\int \left\{(k_x - k_y) 2Re\left[\left(\frac{\partial T}{\partial \xi}\right)^2 \frac{1}{|f'(\xi)^2|}\right] + 2(k_x + k_y)\frac{\partial T}{\partial \bar{\xi}}\frac{\partial T}{\partial \xi}\frac{1}{|f'(\xi)^2|}\right\} |f'(\xi)|^2 r\, dr\, d\theta - \frac{1}{2}\int\int qT|f'(\xi)|^2 r\, dr\, d\theta. \tag{4}$$

Taking now a summation of coordinate functions that satisfy the boundary conditions

$$T \cong T_a = \sum_{i=1}^{N} A_i g_i(\xi, \bar{\xi}, \gamma) \tag{5}$$