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The Combustion of Linear Droplet Arrays in a Coaxial Convective Flow.

Jeng-syan Tsai
Louisiana State University and Agricultural & Mechanical College

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Tsai, Jeng-Syan, Ph.D.
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The Combustion of Linear Droplet Arrays in a Co-Axial, Convective Flow

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and Agricultural and Mechanical College
in partial fulfillment of the requirements for
the degree of Doctor of Philosophy

in

The Department of Chemical Engineering

by

Tsai Jeng-Syan
Diploma, Kaohsiung Institute of Technology
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September, 1990
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ABSTRACT

As approximations for spray-combustion processes, a series of increasingly sophisticated numerical models has been developed to simulate the combustion of linear droplet arrays in a co-axial, convective flow. Common to all of the models is an embedded grid, developed to increase computational accuracy.

The first and simplest model is potential flow model (for Re → ∞). The flow is assumed to be ideal and infinitely-fast kinetics (flame sheet assumption) represent the combustion. The results show that the instantaneous droplet burning rates are increased as the droplet spacing is increased, and the burning rates of droplets tend asymptotically to smaller values as the number of droplets in the array is increased.

A second model, a Stokes flow model (for Re < 1), is developed by using the Stokes approximation for the flow field. The results show that, owing to the lack of strong convective flow, the temperature and species contours can penetrate deeper into the flow.

The third model extends the analysis to heat transfer for linear arrays of spheres at any Reynolds number, i.e. the model is based on the steady-state Navier-Stokes equations, but no combustion is considered. A more accurate flow pattern around the arrays is obtained and the predicted heat transfer and drag agree well with the experimental data in the literature.

The fourth model introduces combustion into the third model through a finite-rate, one-step chemical reaction approximation. The model predicts a thick flame layer, rather than a flame sheet. For large Reynolds numbers, the results show that the downstream droplets have a higher burning rate than the leading droplets. For small Reynolds numbers, the model predicts behavior similar to that predicted with the potential and Stokes flow models.

Finally, an unsteady-state model, based on the full Navier-Stokes equations, is used to study the variation in burning behavior with time. The reduction in droplet size, velocity, and spacing is included. The results show that even when the droplet spacing is significantly reduced (from 14 to 6 radii) the burning behavior of droplets is not affected.
Chapter 1

Introduction

Spray combustion is a key process for many real combustion applications such as incinerators, furnaces, engines, and the like. In order to improve the efficiency of those devices, it is important that we have a good understanding of spray combustion processes. A typical spray combustion process includes: 1) the formation of droplets, 2) the transient heating and vaporization of the droplet, and 3) the ignition and combustion of the vapor. The process is further complicated by the convective heat and mass transfer around the droplets, droplet size differences, internal circulation of liquid within the droplet, and mechanisms of various chemical reactions.

The bulk of recent relevant research has focused on either the burning of single, isolated droplets or the group combustion behavior of the spray. On one hand, single droplet studies are unrealistic because they ignore droplet-droplet interactions. On the other hand, the studies of sprays are expensive and complex, and they are often unrealistic because of the many simplifying assumptions required to make theoretical analyses tractable. As a result, the detailed information on the combustion behavior of an ensemble of droplets is lacking. In this project we propose to bridge the gap between these two extremes by studying the combustion of linear droplet arrays. Our goal is to provide the fundamental information on the behavior of droplet arrays in a combustion environment that is necessary for the improvement of mathematical models for spray combustion. At this time, however, it is infeasible to study the key factors that dominate combustion in a three dimensional spray with large number of droplets. In order to make the problem more manageable, we choose to study one-dimensional, linear droplet arrays with a small number of droplets. For such an array, mathematically, we can take advantage of the symmetry around the array axis and reduce a three-dimensional problem to a two-dimensional one. Experimentally, the linear droplet arrays can be more easily generated and better controlled. The experimental results can then be used to verify the accuracy of various theoretical models.

This study is concerned with, for the most part, a numerical simulation of droplet combustion. A small part of the study is directed toward experimental work. The topics of the dissertation presented as follows.

In Chapter 2, a comprehensive review of recent research in droplet combustion is given. The review includes the progress of the development of mathematical models, as well as experimental work, on the combustion of single-droplet, multiple-droplet, and spray systems.

In Chapter 3, the embedded grid system for our numerical study is described. This system consists of a number of spherical grids embedded in a curvilinear grid. A general concept of generating curvilinear grids, as well as the particular technique for generating the curvilinear grid used in this study, is also given.

In Chapter 4, a relatively simple model to calculate the combustion of linear droplet arrays is presented. In this model, potential flow is assumed. Through this assumption, the calculation of the flow
field can be simplified, and the computational time is greatly reduced. The combustion is approximated by infinitely-fast chemical reactions (flame-sheet approximation). Calculations have been performed for linear arrays with three different droplet spacings, burning at various Peclet numbers.

In Chapter 5, we describe a model used to calculate the droplet burning in a low Reynolds number viscous flow (Re<1). At such low Reynolds numbers, the solution for a linear array of droplets in a creeping flow is available in the literature. Therefore, the solution procedure for this model is relatively easy. This model has been applied to three interacting droplets at two different spacings, as well as to arrays with four droplets.

In Chapter 6, a more sophisticated model is developed to calculate the steady-state heat transfer for a viscous flow around linear, solid-sphere arrays at intermediate Reynolds numbers. In this model, the flow field is governed by the steady-state Navier-Stokes equations, and a numerical scheme SIMPLE is used to solve the pressure-linked momentum equations. The details of SIMPLE are given, and the results of calculations performed for the heat transfer for three-sphere arrays at two spacings and various flow conditions are presented and discussed.

In Chapter 7, a steady-state model for the burning of linear droplet arrays under viscous flow conditions is presented. This model is an extension of the model proposed in chapter 6. Here, however, finite-rate chemical kinetics are used to simulate combustion in the gas phase. This model is used to study the flame structure, species distribution, and local mass burning rate of single droplet and linear arrays with three droplets.

In Chapter 8, the steady-state model in Chapter 7 is extended to an unsteady-state model to simulate the transient behavior of burning droplet arrays. In this model, the droplet sizes and spacings are both varying during the burning process, and an adaptive grid is employed to handle those changes. This model is used to study the time-varying flame structure, droplet-droplet interactions, and the individual lifetime history of each droplet in the array.

In Chapter 9, the results from the simulation models in previous chapters are briefly described and compared to provide a more global view of the advantages and limitations of these models.

In Chapter 10, some future research directions on the combustion of linear arrays are proposed.

In the Appendix A, a brief description of the apparatus developed for parallel experimental work is presented, and recommendations for equipment modifications and experimental procedures are given.
Chapter 2

Literature Review

Most recent research efforts to understand spray combustion can be roughly classified as single-droplet studies, group-combustion studies, and small-number-droplets studies. In this chapter, a literature survey on the progress in these research directions is presented.

The Progress of Single, Isolated-Droplet Studies

Early efforts to understand the combustion of sprays focused on the evaporation and combustion of single, isolated, one-component fuel droplets. Spalding (1953) and Godsave (1953) predicted that the surface area of the droplet decreases linearly with time, which is known as the $d^2$-law. In their model, it was assumed that the transport properties were constant, the Lewis number was unity, the transport processes were quasi-steady, and droplet temperature was uniform.

More sophisticated model have been developed by systematically relaxing the assumptions introduced by Spalding and Godsave. For the spherically symmetric-case, recent development include, but are not limited to, droplet ignition (Rah, Sarofim, and Beer, 1986; Bergeron and Hallett, 1988; Mawid and Aggarwal, 1989), transient droplet heating (Law, 1976a; Dwyer, Kee, Barr, and Sanders, 1983), multicomponent fuels (Law, 1976; Law and Law, 1982; Wang and Law, 1985; Makino and Law, 1988), variable gas-phase transport coefficients (Law and Law, 1977), fuel vapor accumulation (Law, Chung, and Srinivasan, 1980), non-steady gas-phase processes (Crespo and Linan, 1975; Hubbard, Denny, and Mills, 1975; Chao, Matalon, and Law, 1985), finite chemical reaction rates (Saitoh and Nagano, 1980; Chung and Law, 1986; Cho, et al. 1990), and transient conduction and surface regression (Antaki, 1986). Asymmetric models, which account for the boundary-layer-like convective transport processes, have included the effects of circulation within the droplet for single (Prakash and Sirignano, 1980; Patnaik, et al., 1986) and multicomponent (Lara-Urbanejo and Sirignano, 1981; Tong and Sirignano, 1986; Magaridis and Sirignano, 1990) fuels. Calculations of this latter type have been extended for high Reynolds and Peclet numbers (Dwyer and Sanders, 1988). For recent comprehensive reviews of quasi-steady and transient droplet evaporation and combustion, see Williams (1973), Faeth (1977), Law (1982), Sirignao (1983, 1988).

The experimental work carried out recently on the burning of a single droplet can be technically classified into three major categories as 1) captive drop method, 2) supporting sphere technique, and 3) free droplet technique. The captive method, including burning droplets suspended from a fire-resistant tip (Aldred, Patel, and Williams, 1971; Kimura, et al., 1986; Antaki and Williams, 1987) and burning droplets under zero-gravity conditions (Kumagai, 1956; Williams, 1981; Choi, et al., 1988; Cho, et al., 1990; Cho, et al., 1990) are usually applied to study the rate of change of droplet size as a function of time. The supporting sphere technique (Aldred, Patel, and Williams, 1971) involves the use of a ceramic porous sphere into which the fuel is fed by small tube. It is used to study steady-state combustion, flame shape, and flame structure. The free droplet technique, however, is used to study droplet burning under a forced convective flow. A single droplet is produced by suitable generators, such as an electrostatic atomizer.
(Hieftje, 1967), a spinning disc atomizer (Yap, Kennedy, and Dryer, 1984), or a vibrating tube (Green, et al., 1988). Other phenomena of single droplet combustion under current investigation include soot formation (Randolph, and Law, 1986), liquid phase coking (Marrone, Kennedy, and Dryer, 1984), droplet extinction (Chung, and Law, 1986; Hara and Kumagai, 1990), and microexplosions (Yap, Kennedy, and Dryer, 1984; Kimura, et al., 1986; Lee and Law, 1988; Wong, et al., 1990; Chung and Kim, 1990).

The Progress of Group-Combustion Studies

The bulk of experimental evidence indicates that sprays in most practical burners are not the combined effect of many individual burning droplets (Chigier and McCreath, 1974). Rather, "group" combustion of droplet clouds appears to be the dominant mode in all but very dilute sprays. Thus, recent interest has focused on the vaporization of droplet clouds that include the effect of droplet interactions on the vaporization process. Group combustion theories and predictions developed include: spray velocity (Li and Tankin, 1989), spray evaporation (Correa and Sichel, 1982; Bellan and Harstad, 1987a, 1987b; Bellan and Cuffel, 1983), spray ignition (Aggarwal, 1989; Mawid and Aggarwal, 1990), flame propagation (Continillo and Sirignano, 1988; Queiroz and Yao, 1989), spray-flame characteristics (Chiu and Liu, 1977; Williams, Carstens, and Zung, 1978; Botros, Law, and Sirignano, 1980; Chiu and Croke, 1982; Sichel and Palaniswamy, 1984; Annamalai and Ramalingam, 1987; Lee and Sichel, 1988; Yang and Sichel, 1988; Bellan and Harstad, 1990a, 1990b). For recent comprehensive reviews of spray evaporation and combustion, see Faeth (1983) and Sirignano (1988).

Along with the progress of theoretical models, some experimental work on spray combustion has also been undertaken. The current experimental studies of spray combustion includes the formation of droplets (Fulton and Tankin, 1987), droplet size distributions (Mao, Oechsle, and Chigier, 1985), droplet velocity (Yule and Aval, 1989; Edwards and Rudoff, 1990), flame stability (Farag, Arai, and Hiroysu, 1982; Schefer et al., 1989), flame propagation (Myer and Leffebvre, 1986; Chen, Lin, and Sohrab, 1988; Nakabe, Mizutani, and Hirao, 1988), and flame structure (Yule and Bolado, 1984; Lee et al., 1988; Presser, Gupta and Semerjian, 1988; Presser et al., 1990).

The Progress of Small-Number-Droplets Studies

So far, the current spray models have not yet been developed to a point where they can either be used to compare with available experimental data or used as reliable design tools. The deficiency of these proposed models with respect to their application to real systems arises because these models oversimplify many important processes, such as forced convection, droplet-droplet interactions, transient heating of droplets, droplet size differences, internal circulation of droplets, and turbulent effects on the combustion process. Although these processes are essential to spray combustion, they are still not very well understood. In order to obtained information on these key processes, studies intermediate between the combustion of single, isolated droplet and group combustion is therefore needed. These intermediate studies must focus on a small number of droplets, and thus they can be regarded as a study of micro-scale spray combustion. This study of micro-scale spray combustion can provide the detailed information on heat transfer, mass transfer, and hydrodynamics that can not be obtained from the study of group combustion. Also, the effect
of droplet-droplet interactions and the detailed flow pattern in the inter-droplet region, which is unavailable in the study of single, isolated-droplet combustion, could be treated in this intermediate-type study.

For droplets burning in a quiescent oxidizing atmosphere, the combustion of two droplet systems (Umemura, Ogawa, and Oshima, 1981) and multi-droplet arrays (Labowsky, 1980; Marberry, Ray, and Keung, 1984; Labowsky, 1986; Umemura, 1990) have been studied using a potential flow assumption, and the burning rate and flame shape around each droplet was predicted. Despite the potential flow assumption and many other simplifying assumptions that are made in these models, Sangiovanni and Labowsky (1982) obtained good agreement with experimental measurements of droplet burning rates by applying one such simple model to simulate the burning of linear droplet arrays in the absence of convection. For droplets burning in a convective environment, a planar droplet array perpendicular to the flow direction was studied by Shun (1987), who concluded that the droplet interaction decreases as the Reynolds number increases. For droplet arrays in tandem with the flow direction, the present authors proposed a potential flow model (Tsai and Sterling, 1988) to calculate the interaction between the upstream and downstream droplets and to evaluate the convective flow effects on the burning droplet array. Other studies with droplet arrays coaxial with the flow direction are limited to heat transfer or mass transfer studies (Amizadeh, et al., 1974; Tal, Lee, and Sirignano, 1982; Tal, Lee, and Sirignano, 1984; Patnaik, 1986; Chen and Tong, 1988; Raju and Sirignano, 1987); nevertheless, they still provide very useful insight to the combustion problems. For a more complicated system, some of the most recent studies even include a number of parallel droplet arrays to simulate spray combustion processes (Rangel and Sirignano, 1989) or liquid hazard waste incineration (Deplanque, et al., 1990).

The experimental investigations for droplet-droplet interactions were first conducted in the early 1950’s (Rex, Fuhs, and Penner, 1956). These early experiments studied the combustion of suspended droplets in quiescent air at different spacings. Several more recent papers (Fedoseeva, 1972 and Fedoseeva, 1973) have dealt with similar experiments, but with the emphasis on droplets burning in a forced convection. With the progress of the droplet-generating techniques, experiments were conducted for one (Sobro, et al., 1988) and two dimensional arrays (Twardus and Brzustowski, 1978) in which the ignition, droplet burning rate, and the flame propagation of the droplet arrays were studied. However, in these studies, the droplet spacing was fixed. With another technique, which uses a charging ring and a set of high voltage parallel plates, a stream of uniform-sized droplets with variable inter-droplet spacings can be generated. This technique has been used to study droplet trajectory (Mulholland, et al., 1988), droplet-droplet interactions (Sangiovanni and Labowsky, 1982), and soot formation (Bonczyk and Sangiovanni, 1984). The above droplet generation technique has also been developed for use in our experimental study, and the principle of this technique is discussed in the Appendix A.
References


Chapter 3

Grid System and Numerical Scheme

Grid System

In this section, the embedded grid used for the numerical modeling will be discussed in detail. The presentation will be made in the following sequence. First, the general concept of the embedded grid will be briefly shown. Once the concept of the embedded grid is described, the Laplace equations, which are widely used to generate a smooth curvilinear grid, will be discussed. Finally, the particular technique used for generating the curvilinear grid used in this study will be given.

1. The configuration of the embedded grid [1]:

   The grid system used in this study is an embedded-grid system in which a C-type system (the general shape of the grid is that of the letter C) is embedded in another curvilinear grid system. A sketch of the grid is shown in Figs. 1 and 2.

   The process of transforming a non-rectangular embedded grid (Fig. 1) to a rectangular grid (Fig. 2) is termed grid opening, and consists of two stages:

   First, consider the three embedded C-type systems, shown in Fig. 1, that surround the exterior boundaries of the three spheres; the regions inside the contour are shown in Fig. 3. These regions open to the three rectangular portions of the transformed region shown in the lower part of Fig. 2. Note that the entire region representing the sphere in Fig. 1 transforms to a slit in Fig. 2.

   The physical region outside the C-type systems (the curvilinear region) is shown in Fig. 4. This region transforms to rectangles and is fitted to the top of the rectangles corresponding to the inner system along the contours 5-8, 9-12, and 13-16, as shown in Fig. 2.

2. The concept of generating a curvilinear grid system [2]:

   Harmonic functions are convenient to use in the generation of curvilinear grids because they are smooth, they have their minimum and maximum values at the boundaries of the domain, and they change monotonically in the interior of the domain. As a result, the harmonic Laplace’s equation is widely used for grid generation.

   If \( \xi(x,y) \) and \( \eta(x,y) \) are the curvilinear coordinates in the desired grid system (see Fig. 2), then they should satisfy the Laplace equations:
\[ \nabla^2 \xi = 0 \quad (1) \]
\[ \nabla^2 \eta = 0 \quad (2) \]

In practice, lines of constant \( \xi \) and \( \eta \) are used. Since it is easier to specify \( \xi \) and \( \eta \) than to specify \( x \) and \( y \), equations (1) and (2) are transformed to corresponding equations in terms of \( x \) and \( y \).

Partial derivatives of an arbitrary function \( \phi(x(\xi,\eta), y(\xi,\eta)) \) are transformed by

\[
\frac{\partial \phi}{\partial x} = \frac{[(\partial y/\partial \eta)(\partial \phi/\partial \xi) - (\partial y/\partial \xi)(\partial \phi/\partial \eta)]}{J} \quad (3)
\]
\[
\frac{\partial \phi}{\partial y} = \frac{[(\partial x/\partial \eta)(\partial \phi/\partial \xi) - (\partial x/\partial \xi)(\partial \phi/\partial \eta)]}{J} \quad (4)
\]

where

\[
J = (\partial x/\partial \xi)(\partial y/\partial \eta) - (\partial x/\partial \eta)(\partial y/\partial \xi) \quad (5)
\]

is the Jacobian of the transformation.

Using equations (3)-(5), we can express the derivatives of \( \xi \) and \( \eta \) with respect to \( x \) and \( y \) as

\[
\xi_x = \frac{\partial y/\partial \eta}{J} \quad (6)
\]
\[
\xi_y = -\frac{\partial x/\partial \eta}{J} \quad (7)
\]
\[
\eta_x = \frac{\partial y/\partial \xi}{J} \quad (8)
\]
\[
\eta_y = \frac{\partial x/\partial \xi}{J} \quad (9)
\]

Upon substitution of \( \xi_x, \xi_y, \eta_x \), and \( \eta_y \) into equations (1) and (2), the Laplace equations are transformed to:

\[
[(\partial y/\partial \eta)/J]_x - [(\partial x/\partial \eta)/J]_y = 0 \quad (10)
\]
\[
-[(\partial y/\partial \xi)/J]_x - [(\partial x/\partial \xi)/J]_y = 0 \quad (11)
\]
After differentiating and rearranging, the Laplace equations become:

\[ \alpha(\frac{\partial^2 x}{\partial \xi^2}) - 2\beta(\frac{\partial^2 x}{\partial \xi \partial \eta}) + \gamma(\frac{\partial^2 x}{\partial \eta^2}) = 0 \] (12)

\[ \alpha(\frac{\partial^2 y}{\partial \xi^2}) - 2\beta(\frac{\partial^2 y}{\partial \xi \partial \eta}) + \gamma(\frac{\partial^2 y}{\partial \eta^2}) = 0 \] (13)

where

\[ \alpha = (\frac{\partial x}{\partial \eta})^2 + (\frac{\partial y}{\partial \eta})^2 \] (14)

\[ \beta = (\frac{\partial x}{\partial \xi})(\frac{\partial x}{\partial \eta}) + (\frac{\partial y}{\partial \xi})(\frac{\partial y}{\partial \eta}) \] (15)

\[ \gamma = (\frac{\partial x}{\partial \xi})^2 + (\frac{\partial y}{\partial \xi})^2 \] (16)

The system of equations (12)-(16) generates equally-spaced lines inside the domain, due to the strong smoothing effect of the harmonic equations used. In many calculations, however, clustering in certain regions is necessary. In order to control the grid spacing, nonhomogeneous terms known as control functions can be added to the equations. The resulting Poisson equations are

\[ \alpha(\frac{\partial^2 x}{\partial \xi^2}) - 2\beta(\frac{\partial^2 x}{\partial \xi \partial \eta}) + \gamma(\frac{\partial^2 x}{\partial \eta^2}) = P_1 \] (17)

\[ \alpha(\frac{\partial^2 y}{\partial \xi^2}) - 2\beta(\frac{\partial^2 y}{\partial \xi \partial \eta}) + \gamma(\frac{\partial^2 y}{\partial \eta^2}) = P_2 \] (18)

where

\[ P_1 = -J^2 \{(\frac{\partial x}{\partial \xi})P(\xi, \eta) + (\frac{\partial x}{\partial \eta})Q(\xi, \eta)\} \] (19)

\[ P_2 = -J^2 \{(\frac{\partial y}{\partial \xi})P(\xi, \eta) + (\frac{\partial y}{\partial \eta})Q(\xi, \eta)\} \] (20)

\( P(\xi, \eta) \) and \( Q(\xi, \eta) \) are the control functions. This system will also have its minimum and maximum at the boundaries of the domain, if the control functions do not change sign within the domain.

3. The grid generation technique used for present study:

The grid for the present study is generated by a method proposed by Knight [3]. The grid generated
by this method can be either a nearly-orthogonal grid, with total control on the grid size, or an orthogonal grid, with partial control on the grid size. In this study the second option is chosen.

The procedure for generating an orthogonal grid, as proposed by Knight, includes two steps. These are an intermediate transformation and a final transformation.

a. Intermediate Transformation ($\xi(x,y), \chi(x,y)$)

The Poisson equations to be solved can be written as

\[ \ddot{x}(\partial^2 x/\partial \xi^2) - 2 \beta(\partial^2 x/\partial \xi \partial \chi) + \gamma(\partial^2 x/\partial \chi^2) = -j^x \phi \]  

\[ \ddot{y}(\partial^2 y/\partial \xi^2) - 2 \beta(\partial^2 y/\partial \xi \partial \chi) + \gamma(\partial^2 y/\partial \chi^2) = -j^y \phi \]  

where

\[ \ddot{x} = x^2 + y^2 \]  

\[ \ddot{y} = x^2 + y^2 \]  

The forcing function $\phi$ is used to generate an orthogonal grid [3].

The mesh points are equally spaced at the inlet and outlet boundary as an initial guess for the grid (see Fig. 5a). On the symmetry boundary, the mesh point can be specified by the user. On the outer boundary, the mesh points are controlled by the local-orthogonal relation:

\[ x_\xi x_x + y_\xi y_x = 0 \]  

The purpose of the intermediate transformation is to obtain the forcing function and the distribution of mesh point along the outer boundary that are consistent with orthogonality. Also, the mesh of the intermediate transformation can be used as an initial guess for the solution of the final transformation equations. Therefore, the intermediate mesh must be stored for this purpose. The grid generated by the
intermediate transformation is orthogonal and allows arbitrary specification of mesh points along the symmetry boundary. However, there is no control on the mesh spacing in the y direction. In order to introduce good control of the grid spacing in the y-direction, a final transformation is necessary.

b. Final Transformation

The Poisson equations of the final transformation are

\[ \alpha(\partial^2 x/\partial \xi^2) - 2\beta(\partial^2 x/\partial \xi \partial \eta) + \gamma(\partial^2 x/\partial \eta^2) = -f^2((\partial x/\partial \xi)P(\xi, \eta) + (\partial x/\partial \eta)Q(\xi, \eta)) \] (29)

\[ \alpha(\partial^2 y/\partial \eta^2) - 2\beta(\partial^2 y/\partial \xi \partial \eta) + \gamma(\partial^2 y/\partial \eta^2) = -f^2((\partial y/\partial \xi)P(\xi, \eta) + (\partial y/\partial \eta)Q(\xi, \eta)) \] (30)

where the definitions of \( \alpha, \beta, \) and \( \gamma \) are the same as those for eqns. (14)-(16), and the forcing function \( P(\xi, \eta) \) is determined from the intermediate transformation according to

\[ P(\xi, \eta) = \phi(\xi, \chi(\eta)) \] (31)

In general, the function \( \chi(\eta) \) is not known \( a \ priori \). However, since \( \phi(\xi, \chi) \) usually varies smoothly with \( \chi \), satisfactory results are obtained when \( \phi \) is linearly interpolated in the physical plane along the grid line. The Q in eqns (29) and (30) is given as:

\[ Q = \frac{\gamma s}{J^2} \] (32)

where

\[ s = T \frac{x_\eta R}{x_\xi y} \text{ if } x_\xi \neq 0 \] (33)

\[ s = T \frac{y_\eta R}{y_\xi x} \text{ if } y_\xi \neq 0 \] (34)

and

\[ T = -(x_\eta x_\eta + y_\eta y_\eta)/(x_\xi^2 + y_\xi^2) \] (35)

\[ R = x_\xi y_\eta - y_\xi x_\eta \] (36)

which result from applying local orthogonality \( \beta = 0 \) in equations (29) and (30).

The boundary condition on the outer boundary is taken from the intermediate transformation, and the mesh points at the inlet and outlet can be specified here by the user. The initial-guess solutions \( x \) and \( y \),
used for the final transformation, are the linear interpolations of the solutions for $x$ and $y$ in the intermediate transformation.

A simple example of applying this grid technique is shown in Fig. 5. Figure 5a is the initial guess of $x$ and $y$ for the intermediate transformation. Notice that along the inlet and outlet, the grid size is uniform, while along the symmetry boundary the grid size is not uniform (it is specified by the user). Fig. 5b shows the intermediate transformation of the grid. It can be seen in this figure that the grid size along the inlet and outlet remains uniform. The grid points along the outer boundary, however, are redistributed to satisfy the local orthogonality relation. By redistributing the grid size along the inlet, and linearly interpolating the solution of $x$ and $y$ in the intermediate transformation as the new initial guess, the final transformation can be obtained by solving equations (29) and (30). The results are shown in Fig. 5c. From this figure, it can be seen that we not only have a very smooth grid distribution in the interior, but we also have a good control of the grid size as well.

**Numerical Scheme**

In this work, the conservation equations that need to be solved in the potential flow model (Chapter 4) and Stokes' flow model (Chapter 5) are the energy and species equations. In models such as the heat transfer model in a viscous flow (Chapter 6), steady-state droplet combustion model (Chapter 7), and unsteady-state droplet combustion model (Chapter 8), the momentum equations need to be solved as well. The numerical scheme SIMPLEM[2] is used to solve the governing momentum, energy, and species equations. However, for the models that do not require a solution to the momentum equations, only the energy and species solvers in SIMPLEM are used. The details and the procedures of the numerical scheme SIMPLEM are shown in Chapter 6 or can be found in Ref. 2. Therefore, they are not repeated here.
References


Figure 1. Sketch of a embedded grid.

Figure 2. Transformation for the grid shown in Figure 1.

Figure 3. The inner domains of the embedded grid shown in Figure 1.

Figure 4. The outer domain of the embedded grid shown in Figure 1.
Figure 5a. Initial guess for the example.

Figure 5b. Intermediate transformation for the example.

Figure 5c. Final transformation for the example.
Chapter 4

The Combustion of a Linear Droplet Array in a Convective, Co-Axial Potential Flow

(submitted to *Combustion and Flame*)
The Combustion of a Linear Droplet Array in a Convective, Co-Axial Potential Flow

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ABSTRACT

An efficient numerical scheme is introduced to describe the effects of forced convection and droplet-droplet interactions on the burning rate of a one-dimensional droplet array. The flow field is described by point sources (or sinks) superimposed on a uniform, coaxial potential flow. The strengths of the sources (or sinks) are found from the mass and heat conservation boundary conditions at the droplet surfaces. The resulting flow field is then used to solve the energy and species conservation equations, which are first transformed to a generalized coordinate system so that the computations can be carried out in any grid system.

In this study, an improved, composite, body-fitted grid was used to solve the equations by an iterative, finite difference method to obtain the temperature (or concentration) field. Droplet pairs of equal sizes with spacings from 4 to 16 radii have been investigated for Peclet numbers from 10 to 120. The temperature distribution around the droplet array, as well as the local Nusselt number around the droplet surfaces, has been calculated. The results show qualitative agreement with analogous heat and mass transfer analyses that have appeared in the literature. Two droplets of unequal sizes and an array of up to six equal sized droplets have also been studied.

This simple approach for treating the flow field allows the computation to be extended to a linear array with a large number of droplets. The numerical scheme has excellent convergence behavior, and the composite grid introduced here can also be used for more accurate, viscous flow calculations.
Introduction

Liquid spray combustion is a complex process. Some of the important features involved include the relative motion between the gas and droplet leading to convective heat and mass transfer, droplet-droplet interactions, and transient heating of the liquid. In order to predict rate processes for droplet combustion, an understanding of these phenomena is essential.

The interactions among droplets in a burning spray, which reduce evaporation and combustion rates compared to the single droplet case, have been demonstrated experimentally. Rex et al. [1] have shown that interaction between two droplets depends on the distance between them. Sangiovanni and Labowsky [2] have found that the burning time of monodisperse droplets in a linear array monotonically increases with decreasing droplet spacing.

Several theoretical approaches have been developed to model the multiple droplet system burning in a quiescent oxidizing atmosphere. Umemura et al. [3] obtained the burning rate and the flame surface shape for pairs of burning droplets by solving the equations for energy and mass conservation in bispherical coordinates. For multiple droplet systems, a model based on the method of images was developed by Labowsky [4]. An easier method was introduced by Marberry et al. [5]. In their method, the burning rate of droplets in an array was calculated using a modified Laplace equation with point sources. However, this approach can not be applied to some extreme cases, as has been discussed by Labowsky [6]. All the above methods are based on ideal flow assumptions.

For droplets burning in a convective environment, Fernandez [7] developed a theoretical model for a single fuel droplet in a forced convection, oxidizing gas flow by making use of boundary layer and flame sheet approximations. Two models were successfully developed by Tal et al. [8,9] to describe the heat and momentum transfer of a multisphere array. One [8] is based on a multisphere cylindrical cell model, which can be applied to an N-sphere system, while the other [9] is developed in bispherical coordinates applicable only to two-sphere systems. These two models are applied only to heat transfer problems but still provide a very useful insight into the numerical solution for mass transfer (evaporation) between the gas phase and the condensed phase in a sphere assemblage. More recently a new grid system has been used by Chen et al. [10] to improve Tal’s model, and better results have been reported.

For droplets evaporating in a high temperature stream, some preliminary work by Yuen et al. [11] provided the basis for Shuen [12] to calculate the combustion of a planar droplet array oriented perpendicular to the approaching flow. Due to the symmetric arrangement and uniform size of the droplets, calculations were required only around a single droplet; the interactions do not include the effects of upstream and downstream droplets. Shuen concluded that the interaction effect on the gasification rate is significant only at small spacing and low Reynolds numbers.

In view of the significant interaction between upstream and downstream droplets demonstrated by Tal [8] and Chen [10], a linear droplet array burning in a convective flow coaxial with the array should be studied to improve our understanding of droplet-droplet interactions in combustion processes.
absence of flow-direction symmetry, the solutions must include the influence of each droplet in the array. The geometric complexity and large computer time and storage needed for numerical calculations have precluded modeling of this important combustion problem for large droplet-number systems. In the present study, an extension of Tal’s work has been used to obtain initial numerical results for a linear droplet array burning in a convective flow parallel to the array axis. As the flow is assumed to be irrotational, the results will be strictly applicable only for large Reynolds numbers. The arrays studied include both droplets of uniform size and droplets of different size.

Mathematical Formulation

1. Assumptions

The gas-phase processes are assumed to be at steady state. This assumption is justified by the large density ratio between the liquid and gas phases. Because of the density difference, the surface boundary, surface temperature, and liquid-phase species concentrations change at a rate much slower than parallel processes in the gas-phase [12]. The effects of condensed-phase internal circulation and transient heating are assumed to be negligible. For a single component fuel at low or moderate ambient pressure, Law [13] and Sirignano [14] have indicated that the transient heating constitutes only a small fraction of total interphase energy transport after the initial 10 to 20 percent of the droplet lifetime. Furthermore, the combustion conditions are considered to be away from ignition or extinction, so that the flame sheet approximation can be applied to describe the gas-phase reactions. In addition, several simplifying assumptions are made as follows:

1. The Lewis number (Le = \( \rho D C_p / k \)) is equal to unity for all chemical species.
2. The spherical shape of each droplet is maintained throughout its combustion.
3. Natural convection and radiative energy transfer are negligible.
4. The temperature is uniform in each droplet and local thermodynamic equilibrium always exists at the surface of each droplet.
5. Physical properties, such as thermal conductivity and gas density, are constant and all species have the same heat capacity and diffusion coefficient.

It should be mentioned that the constant overall gas density assumption is essential for the present study because the constant overall density allows the classical stream function-potential solution of Laplace equation to be used for the flow field calculation. The same constant overall gas density assumption has also been used in another recent combustion study [15]. However, the assumption that the other physical properties are constant and the flame-sheet assumption are not essential to the present analysis and can be relaxed for more detailed combustion studies. The major reason to use these assumptions is to simplify the computation procedure and save computational time.
2. Governing Equations

The linear droplet array in the present analysis is confined in a multispherocylindrical cell, as shown in Fig. 1, and the equations of conservation of mass, energy, and species for the axisymmetric flow in cylindrical coordinates are:

\[
\frac{\partial u}{\partial x} + \frac{1}{y} \frac{\partial (yu)}{\partial y} = 0 \tag{1}
\]

\[
\frac{\partial}{\partial x} (\rho C_p u y T) + \frac{\partial}{\partial y} (\rho C_p vu T) = \frac{\partial}{\partial x} (ky \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (ky \frac{\partial T}{\partial y}) + yq \tag{2}
\]

\[
\frac{\partial}{\partial x} (\rho y Y_i) + \frac{\partial}{\partial y} (\rho vu Y_i) = \frac{\partial}{\partial x} (\rho D_y \frac{\partial Y_i}{\partial x}) + \frac{\partial}{\partial y} (\rho D_y \frac{\partial Y_i}{\partial y}) + ym_i; \ i=f,o \tag{3}
\]

with the boundary conditions:

a. at the inlet

\[ T = T_\infty \]

\[ Y_o = Y_o,\infty \]

\[ Y_f = 0 \]

b. on the cylindrical envelope

\[ \frac{\partial T}{\partial x} = 0 \]

\[ \frac{\partial Y_i}{\partial x} = 0; \ i=f,o \]

c. on the sphere surface

\[ T = T_w \]

\[ k \frac{\partial T}{\partial n}_w = (\rho U_n)_w L_v \]

\[ Y_o = 0, \ Y_f = (Y_f)_w \]

d. along the axis of symmetry

\[ \frac{\partial T}{\partial y} = 0 \]

\[ \frac{\partial Y_i}{\partial y} = 0; \ i=f,o \]

e. at the outlet

Equations (2) and (3) can be written in the Schwab-Zeldovich form as:

\[
\frac{\partial}{\partial x} (\rho C_p u y F) + \frac{\partial}{\partial y} (\rho C_p vu F) = \frac{\partial}{\partial x} (ky \frac{\partial F}{\partial x}) + \frac{\partial}{\partial y} (ky \frac{\partial F}{\partial y}) \tag{4}
\]

\[
\frac{\partial}{\partial x} (\rho y F') + \frac{\partial}{\partial y} (\rho vu F') = \frac{\partial}{\partial x} (\rho D_y \frac{\partial F'}{\partial x}) + \frac{\partial}{\partial y} (\rho D_y \frac{\partial F'}{\partial y}) \tag{5}
\]

with coupling function \( F \) and \( F' \) defined as [7]:

\[
F = \frac{C_p (T - T_\infty)}{L_v} + \frac{(Y_o - Y_o,\infty)Q}{M_o v_o L_v}
\]

\[
F' = \frac{Y_o Q}{M_f v_f L_v} + \frac{(Y_o - Y_o,\infty)Q}{M_o v_o L_v}
\]
The coupling functions $F$ and $F'$ are linearly related. When an infinitely fast reaction rate (flame sheet approximation) is assumed, the following relation holds [7]:

$$F' = -(1 + \gamma) QF / [(1 + B) M_f v_f L_v]$$

where

$$\gamma' = Y_0 v_f / M_f v_0$$

$$B = [(Y_0 v_0 Q / M_f v_0) - C_p (T_w - T_\infty)] / L_v$$

Since $F$ and $F'$ are linearly related, only $F$ is calculated in the present analysis.

3. Flow field calculations

We introduce the potential function as

$$u = \frac{\partial \phi}{\partial x} \quad v = \frac{\partial \phi}{\partial y}$$

In terms of the potential function, the continuity equation reduces to the Laplace equation:

$$\frac{1}{y} \frac{\partial \phi}{\partial y} + \frac{\partial^2 \phi}{\partial x^2} = 0 \quad (6)$$

Based on the linearity of the Laplace equation, the solution for an axisymmetric flow around a body of arbitrary shape can be constructed by superimposing the field of a uniform stream and the fields of a series of point sources located within the body with strengths chosen in such a way that the appropriate boundary conditions at the body surface are satisfied [16]. The same principle is applicable to a multibody system. In the present study, $N$ point sources are placed along the $x$ axis as shown in Figure 2. With a superimposed uniform flow in the $x$ direction, the general solution of Eq.(6) can be written as:

$$\phi = \sum_{j=1}^{N} \frac{g_j}{r_{ij}} + U_w r_i \cos \theta \quad (7)$$

where the $g_j$ are the unknown source strengths inside the droplets, $N$ is the number of point sources, $r_{ij} = (x_i - x_j)^2 + (y_i - y_j)^2$, $r_i^2 = x_i^2 + y_i^2$, $U_w r_i \cos \theta$ is the potential of the uniform stream, and $\theta$ is the polar angle. The fact that a point source and the uniform stream are solutions of the Laplace equation can be easily verified by substituting them individually into Eq. (6).

As $r_{ij} \to \infty$, $\phi$ approaches the potential of the uniform stream. Hence the boundary condition at the region far away from the droplets is satisfied identically.

On the droplet surfaces, we have

$$k \left( \frac{\partial T}{\partial n} \right)_w = (\rho U_w)_w L_w = \rho \left( \frac{\partial \phi}{\partial n} \right)_w L_w \quad (8)$$

where $L_v$ is the heat of vaporization and $k$ is thermal conductivity of the gas. The substitution of Eq.(7) into Eq.(8) is applicable to $M$ locations on each droplet surface when $M$ point sources are used in each droplet, and a system of $(K \times M)$ equations is generated for a system of $K$ droplets in the array. One can
solve for $K \times M$ unknown source strengths from the $K \times M$ equations. Once these source strengths are obtained, the stream function and the velocity of the flow field can be obtained from the potential function [17]. The stream function is defined as:

$$\psi = \frac{1}{y} \frac{\partial \psi}{\partial x} \quad \nu = \frac{1}{y} \frac{\partial \psi}{\partial y}$$

4. Transformation of Governing Equations

In order that the computations can be performed on a rectangular grid in the computational plane, it is necessary to transform the governing equations from the physical domain $(x,y)$ to the computational domain $(\xi, \eta)$. When transformed into new independent variables $\xi$ and $\eta$, Eq.(4) changes according to the general transformations $\xi = \xi(x,y)$ and $\eta = \eta(x,y)$. Partial derivatives of the function $F$ are transformed according to

$$F_x = (y_\eta F_\xi - y_\xi F_\eta)/J \quad \text{and} \quad F_y = (-x_\eta F_\xi + x_\xi F_\eta)/J$$

where $J$ is the Jacobian of the transformation given by

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Upon introducing

$$G_1 = u y_\eta - v x_\eta, \quad G_2 = v x_\xi - u y_\xi$$

$$\alpha = x^2_\eta + y^2_\eta, \quad \beta = x_\xi x_\eta + y_\xi y_\eta, \quad \text{and} \quad \gamma = x^2_\xi + y^2_\xi$$

Eq. (4) can be transformed to:

$$\frac{\partial}{\partial \xi} (G_1 y F) + \frac{\partial}{\partial \eta} (G_2 y F) = \frac{\partial}{\partial \xi} [(\Gamma y/J)(\alpha F_\xi - \beta F_\eta)] + \frac{\partial}{\partial \eta} [(\Gamma y/J)(\gamma F_\eta - \beta F_\xi)]$$

where

$$\Gamma = (k/\rho C_p)$$

5. The Choice of Grid

The numerical solution of any partial differential equation requires the discretization of the computation domain; therefore, grid generation is the first step in the solution procedure. Two major features studied in the present analysis are the droplet-droplet interaction and the burning rate at the droplet surfaces. Therefore, the grid for numerical calculations was chosen carefully so that these two major features could included and investigated accurately.

For a convective flow around a linear droplet array, the multisphere cylindrical cell is often used to tackle the problem. The multisphere cylindrical cell was first introduced by Tal et al. [9]. In their work, they used a non-uniform, cylindrical polar mesh as indicated in Fig. 3. The problem associated with this
grid is that the nodes on the sphere surface are not distributed uniformly. Thus the accuracy of the solution will be affected. Also, around the sphere surface, the streamlines cut diagonally across the grid, which might be the source of false diffusion reported in some work [18].

A new grid system, as shown in Fig. 4, generated by solving elliptic partial differential equations, was adopted by Chen et al. [10] to eliminate the disadvantage of the above mesh. In their work, the grid is distributed more uniformly around the sphere surface. The mesh around the sphere surface, however, is not orthogonal and the distance between the nodes next to the surface and the surface nodes is not uniform. These missing characteristics limit the ability to evaluate accurately the gradients around the sphere surface.

The complexity of the geometry of the multisphere cylindrical cell and grid systems discussed above, implies that it is almost impossible for a single mesh system to fit the complicated geometry of the multisphere cylindrical cell and still provide all the desired features for the sphere surfaces. Furthermore, when evaporation is occurring at the droplet surface, the normal velocity is proportional to the temperature gradient. In order to evaluate accurately the temperature gradient, the grid should be fine and orthogonal around the droplet surface. Therefore, a composite mesh should be the next reasonable candidate for a better grid system. Launder and Massey [18] suggest a composite grid, where the drawbacks of previous work have been largely eliminated. Although their approach is for flow over a tube bank, the same idea can also be applied for the multisphere cylindrical cell. Close to the sphere, a spherical grid is retained and the remaining flow region is filled with a uniform cylindrical polar mesh, as shown in Fig. 5. This composite grid system, although it can eliminate most drawbacks of a single mesh system, presents a very complex situation at the intersection between the polar grid and the spherical grid and requires a very tedious calculation along this intersection. A similar difficulty is also encountered with the grid proposed by Pataink [19], which uses two overlapped spherical meshes to calculate the droplet history of two interacting and evaporating droplets.

In the present study, an embedded grid (see Fig. 6) is used and is found to be adequate for both droplet interactions and evaporation (or combustion) studies for a linear multi-droplet array. In the embedded grid, a spherical mesh is used around each droplet surface and the rest of flow region is covered by a nearly orthogonal curvilinear mesh, generated by the method developed by Knight et al [20]. Based on the solution of Poisson's equations, this technique is capable of generating either orthogonal grids with partial control of the mesh spacing or nearly orthogonal grids with full control of the mesh spacing. In this work, we use the first of these options. Since the orthogonality is not required in the outer domain, however, any other appropriate technique can be used to generate the outer curvilinear mesh.

The performance of the proposed embedded grid has been tested by repeating some of the calculations by Aminzadeh, et al [21]. In their work, the mass transfer between two droplets at low Reynolds number but high Peclet number were computed by using bipolar coordinates. The results of our computations [22] agree very well with their published data. We are therefore confident that our grid system can be applied to the present combustion study.
Solution Procedure

With the grid system described in the last section, the computational domain can then be as shown in Fig. 7a. Figures 7b and 7c show the transformed calculation domain and the boundaries (meshed area) for the curvilinear mesh and spherical mesh respectively. The calculations in the two domains are carried out separately. It can be seen from Figure 7b that one row of the interior nodes in the spherical mesh serves as a boundary condition for the calculation of the curvilinear mesh; figure 7c indicates how the intersection between the curvilinear mesh and the spherical mesh serves as a boundary condition when the calculations are performed in the spherical mesh. It should be mentioned that the slab corners in the transformed domain are points which require special treatment. In this study, the values of the special points were obtained by linear interpolation between the neighboring nodes along the axis of symmetry in the physical domain. Other techniques for treating the special point can be found in reference [23].

In order to perform the numerical computation, the transformed conservation equation (9) can be integrated over a finite control volume around each node in the grid system discussed above to form a set of algebraic equations. A power-law scheme is used during the integration in the present study. The details of the integration and the resulting algebraic equations can be found in references [24] and [25]. Therefore they are not repeated here.

The procedure to solve for the coupling function $F$ is summarized below:

1. Start with a assumed value of $F$ at all internal nodes.

2. Use the values of $F$ on the droplet surface, together with values of $F$ on the adjacent nodes in the normal direction from the droplet surface, to approximate the temperature gradient in Eq. (8), and solve the system of $K \times M$ equations for the source strengths $g_r$.

3. Use the known source strengths calculated in step 2 to determine the flow field with Eq.(7). The potential function can then be transformed to the corresponding stream function to calculate the flux over the faces of the control volumes around each node.

4. With the flow field known, the coefficients in the system of algebraic equations can be determined, and the system of equations can then be solved with line-by-line TDMA [25] to obtain a new $F$ field.

5. With the new $F$ field as an improved guess, repeat steps 2 to 5 until convergence is achieved.
Results

Illustrative calculations have been carried out for polymethylmethacrylate (PMMA) droplets burning under atmospheric conditions. A solid fuel was selected because internal circulation is neglected in the analysis. The following properties, similar to those used by Fernandez-Pello [7] were used in the calculation:

\[
C_p = 0.4516 \text{ cal/g } \text{o} \text{C} \\
k = 12.96 \times 10^{-5} \text{ cal/cm s } \text{o} \text{C} \\
\rho = 0.8949 \times 10^3 \text{ g/cm}^3 \\
L_v = 380 \text{ cal/g} \\
Q = 3244 \text{ cal/g of oxidizer} \\
\nu_o/\nu_p = 6 \\
T_w = 663 \text{ oK} \\
T_w = 298 \text{ oK} \\
M_p = 100 \\
M = 32
\]

Numerical solutions of the conservation of energy equation were obtained for three different droplet spacings and Peclet numbers in the range of 10 to 120. The study also includes a system of six equal size droplets as well as a system with droplets of different size.

The number of point sources needed for each droplet was also studied. Theoretically, the gasification rate on the droplet surface will be better described if more point sources are used. However, a larger matrix will result, which will require more computer time for the solution and sometimes preclude the study of large number droplet systems. It was found that nine point sources provided sufficient accuracy for all cases in this study. Figure 8 shows the comparison of the local Nusselt number on the droplet surfaces for calculations with nine point sources and 21 point sources. The local Nusselt number here is defined as:

\[
Nu = \frac{(2Rh/k)}{(\theta_f - \theta_w)}
\]

where

\[
h = \frac{(k \frac{dT}{dn})_w}{(T_{flame} - T_w)}
\] (10)

and R is the drop radius. It can be seen that very little difference can be detected. Therefore, nine point sources were placed within each droplet through out the rest of this study. It should be mentioned that:

1. In order to avoid an infinite point source, no source should be placed too near the front stagnation point (or rear stagnation point.) It is found that a distance greater than 0.1 droplet diameter from these points will always gives meaningful results.

2. When the number of point sources within each droplet is less than the number of nodes on the droplet surface (up to 21 in this analysis), the locations at which Eq. 8 is applied on the droplet surface should spaced as evenly as possible to give a good representation of the evaporation rate on the entire droplet surface.
Figures 9 and 10 show the temperature contour lines for two droplets burning in a uniform stream with a Peclet number of 90. The dimensionless distances between the centers of the two droplets are 8.0 and 16.0 respectively. The flame temperature and the flame sheet location can be determined by the formulation shown in reference [7]. The flame temperature for this calculation is 1700 K. It is located at the third contour line, counting from the outermost contour line. Note particularly the trends that can be observed from these two figures. In Fig. 9, the fifth contour line (from the outermost) enclose both the upstream and downstream droplets. As the droplet spacing increases from 8 to 16 radii, i.e. Fig. 10, these same contour line encloses each droplet individually. If this trend is continued to larger droplet spacing, the flame sheet will pinch off resulting in individual droplet flames. This result agrees well with preliminary experimental observations we have made for linear droplet arrays burning in a cross flow.

A two-droplet system was studied to demonstrate the temperature profile variation with Peclet number and the center to center distance between the droplets. The local Nusselt numbers obtained from Eq. (10) were plotted vs. the angle from the front stagnation point, with Peclet number as a parameter, and are shown in Figs. 11-13. For L/R=16, Figures 11a and 11b show that the higher the Peclet number the higher the Nusselt number on the droplet surface. This is due to the decrease of the distance between the flame sheet and the droplet surface: Because the two droplets are very far apart, the curves for each droplet are very similar and resemble the curves for single isolated droplets. However, the magnitude of the local Nusselt number is somewhat lower for the downstream droplet than for the upstream droplet owing to the presence of some unburnt fuel from the upstream droplet around the downstream droplet. These unburnt fuel vapors, carried downsteam by convective flow, tend to reduce the temperature around the downstream and cause the burning rate of the downstream droplet to decrease.

For L/R=8.0, the local Nusselt number curves are shown in Figures 12a and 12b. For the upstream droplets, the local Nusselt number curves for each Peclet number are almost identical for the two different droplet spacings. For the downstream droplets, however, the values of the Nusselt number at the front stagnation point are appreciably lower at this smaller spacing, but they fall off more slowly around the sphere to reach nearly the same value at the rear stagnation point as was observed with the larger spacing discussed above. The more severe retardation of local Nusselt number around the front hemisphere of the downstream droplet are owed to the presence of relatively cold, unburnt fuel in the vicinity of the downstream droplet.

For L/R=4.0, the smallest droplet spacing studied in this work, the local Nusselt number curves are shown in Figures 13a and 13b. The Nusselt number of the upstream droplet remains quite the same as observed for larger spacings. However, for downstream droplets the behavior is quite different. The Nusselt number is very low at the front stagnation point, rises to a maximum at about 60 degrees, and then falls off again until the rear stagnation point is reached. This effect is due to the greatly reduced temperature gradient around the front hemisphere of the downstream droplet, so that little heat transfer from the droplets can occur. It is clearly seen from these results (when compared to the results for L/R=8.0), that interaction between droplets is increased as the droplet spacing is decreased.
The overall average Nusselt number for the droplet, calculated as

\[ \overline{Nu} = \frac{1}{2} \int_{0}^{\pi} Nu \sin \theta' d\theta' \]

where \( \theta' \) is the angle from the forward stagnation point, is plotted vs. Peclet number in Figs. 14-16. For the largest droplet spacing, the curves (Fig. 14) for each of the two spheres are closer together, which indicates a relatively small interaction between them. As the spacing between the droplets is decreased, the overall Nusselt number for the downstream droplet also decreases at any fixed Peclet number, showing the increasing interaction effects on the transfer processes.

In most of the existing literature, the number of spheres included in a linear is very limited (less than three). In order to understand the droplet behavior at locations far downstream, calculations have been performed for 6 droplets with \( Pe=120 \) and \( L/R=4.0 \). The local Nusselt numbers are shown in Figure 17. It can be seen the Nusselt number curve of the first droplet remains unchanged, but for the second droplet the magnitude of the Nusselt number is greatly reduced, indicating a reduced combustion rate. It can also be seen that the pattern of the curves of Nusselt number of the downstream droplets gradually converge to a single pattern far downstream. For droplets 5 and 6, there is very little difference between their Nusselt number curves. This asymptotic behavior allows us to deduce the local Nusselt number for any droplet in infinite array.

Figure 18 shows the resulting Nusselt number for two pairs of droplets, one with uniform size the other with a different size. The diameter of the larger (downstream) droplet (=2R) is used as the characteristic length for the Peclet number and local Nusselt number. It is found that when the size of the upstream droplet is reduced, it has both a higher heat transfer rate and less influence on the downstream droplets.

Discussion

The Method of Images (M.O.I.), a model also based on the potential flow assumption, has been proposed by Labowsky [2,4,6] and been used to calculate the burning time of linear droplet arrays burning at the absence of convective flow. The results show good qualitative agreement with the experimental trends [2]. The only difference between our model and the M.O.I. is that convective flow is included in our model. Therefore, our model can be regarded as an improvement of the M.O.I.. If the convective flow is turned off, the present model is identical to the model proposed by Labowsky. Since the M.O.I. has proven adequate to simulate the burning time of linear droplet arrays burning at the absence of convective flow, the same qualitatively agreement will be obtained if the present model is used to simulate the same experiment.

Attempts have been made to find experimental results for droplets burning in a convective flow in order to compare with the present numerical results. Unfortunately, no applicable experimental results have been found. The numerical results from reference [3], [8], [9], [10], and [21] have been used, however, to provide a qualitative comparison to the results of present study.
The mass transfer between two droplets, for four different Peclet numbers and four different spacings has been investigated by Aminzadeh, et al. [21] and the heat transfer between two droplets, for a Reynolds number equal to 40 and two small droplet spacings has been studied by Tal et al. [9]. Comparing our results with the results of Aminzadeh, it is found that the shape of the curves for the overall average Nusselt number (or Sherwood number) against Peclet number have same general shape, but our magnitudes are about two fold larger for both the upstream and downstream droplets in the Peclet number range from 10 to 50. The difference in magnitude owes to the inclusion of combustion in the present study. For large droplet spacing, the shape of the local Nusselt number curves is very similar to the local Sherwood number curves determined by Aminzadeh for both the upstream and downstream droplets. For small droplet spacing, it is observed that the local Sherwood number curves in Aminzadeh's work and the local Nusselt number curves in Tal's work for the upstream droplet are steeper than the corresponding curves for an isolated droplet (or an upstream droplet with large spacing.) This behavior is not observed in the present results, even with the smallest droplet spacing studied. A possible reason for this difference may be that viscous effects are not considered in this study; therefore, the wake effect, which reduces the heat and mass transfer rate behind the upstream droplet, is neglected. However, the influence of the downstream droplet on the wake of the upstream droplet, and thus on the overall Nusselt number of the upstream droplet, is shown by Tal to be almost insignificant for the droplet spacings used here. Specifically, Tal found that the overall Nusselt number of an upstream droplet, which is almost in contact with the downstream droplet, is 85 percent of a single isolated droplet, while the overall Nusselt number of an upstream droplet separated from the downstream droplet five radii, is 95 percent of a isolated droplet. For downstream droplets, the curves of local Nusselt number found in the present study agree qualitatively with the results of both Aminzadeh and Tal.

For an array with more than two droplets, the results from Tal [8] and Chen [10], where only three droplets are considered, have been used for comparison with the present six-droplet case. The local Nusselt number curves for the first three droplets exhibit a very similar pattern to those found in the present study. No asymptotic behavior is observed for the first three droplets in their work; this agrees with the present results. However, an asymptotic behavior does emerge in this study for an array with more than three droplets.

For a two-droplet array with droplets of different size, the results of Umemura, et al. [3], which include two burning droplets with different size in a quiescent oxidizing atmosphere, has been compared to the present results. In Umemura's work, forced convection was not included and the local burning rate (or local Nusselt number) was not calculated. However, it can be deduced from their results that the influence of one droplet on a second decreases with droplet size. This trend agrees with the present results, and can be easily justified by imaging the limiting case of one droplet becoming vanishingly small so that the other droplet is not affected at all. Thus, the conclusion that smaller droplet give less influence on the other droplet is reasonable.

The above comparisons indicate the results of the present study agree well with the general features of analogous heat and mass transfer studies on linear sphere arrays reported in the literature. We have also attempted to make quantitative comparisons between the present results and the results in the literature.
However, because combustion is included in the present potential-flow study and viscous effects in the absence of combustion are considered in the existing literature, no quantitative comparison is possible at this stage.

Summary

An easy and economical method is introduced to calculate the combustion of interacting droplets in a linear array. In order to isolate the effect of droplet spacing on the droplet-droplet interaction, only pseudo steady-state droplet combustion is considered in this study. Instead of solving the momentum equations in Navier-Stokes form, the flow field is described by point sources superimposed on a uniform, irrotational flow. The equations of conservation are solved in a composite, body-fitted grid. Numerical solutions have been obtained for a Peclet number range of 10-120 and three different droplet spacings. A system with 6 droplets and a system with different droplet sizes are also included.

The flame sheet assumption, potential flow assumption, and the constant transport properties used in this study can be systematically relaxed to provide a model with the potential for detailed combustion studies. However, providing the results of such intensive calculation is not the purpose of present study. Although some work has been done in this area [26], it is found the computer time and storage is overwhelmingly large. For example, because of the slowness of reaching a converged solution and the tedious calculation required for the transport properties, the typical computational time required for a detailed combustion study is around 30 to 60 times more than the current model. Furthermore, the calculation procedure for the detailed combustion is far more complicated. Therefore, the present model can provide an easier and more economical computation for burning linear droplet arrays.

For spray combustor analysis, a droplet is usually considered as a point source of mass. However, when droplet size is not negligibly small compared to mesh sizes, and when vaporization occurs in a convective flow, where the spherically symmetry assumption is not valid, a potential error occurs. In this analysis the concept of placing a series point sources within each droplet and then superimposing a free stream upon these sources is a potential solution to remedy the potential error in present spray combustor analyses. The accuracy of the flow calculations can be improved by increasing the number of point sources. For a large number of droplets, the number of point sources used can be reduced to save computer time. Therefore, the use of the point sources is problem dependent. It is hoped that this feature will provide some useful insight for the large number of droplets that must be included in any reasonable spray analysis.

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References


Nomenclature

\begin{itemize}
\item B \quad \text{mass transfer number}
\item C_p \quad \text{mean specific heat}
\item D \quad \text{diffusion coefficient}
\item F, F' \quad \text{Shvab-Zeldovich coupling functions}
\item G_1, G_2 \quad \text{convective term normal to the grid cell boundary}
\item h \quad \text{heat transfer coefficient}
\item k \quad \text{thermal conductivity}
\item L \quad \text{distance between the centers of two spheres}
\item L_e \quad \text{effective heat of evaporation}
\item Le \quad \text{Lewis number}
\item M \quad \text{molecular weight}
\item m \quad \text{volumetric mass generation rate in gas phase reaction}
\item N \quad \text{total number of point sources}
\item n \quad \text{normal to the sphere surface}
\item Nu \quad \text{local Nusselt number}
\item Nu \quad \text{overall average Nusselt number}
\item Pe \quad \text{Peclet number } (=2RU_0/T)
\item q \quad \text{volumetric heat released in gas phase reaction}
\item Q \quad \text{heat of combustion per gram of oxidizer}
\item R, R' \quad \text{radius of droplets}
\item r_{ij} \quad \text{distance between point } i \text{ and the point source } j
\item r_i \quad \text{distance between point } i \text{ and the origin}
\item T \quad \text{temperature}
\item U \quad \text{velocity}
\item u, v \quad x \text{ and } y \text{ components of velocity}
\item Y_i \quad \text{mass fraction of species } i
\item x, y \quad \text{axial and radial coordinates}
\end{itemize}

\textbf{Greek}

\begin{itemize}
\item \alpha, \beta, \gamma \quad \text{coordinate transformation parameters}
\item \gamma' \quad \text{mass consumption number}
\item \upsilon \quad \text{stoichiometric coefficient}
\item \xi, \eta \quad \text{natural coordinates}
\item \Gamma \quad \text{thermal diffusivity } (=k/pC_p)
\item \rho \quad \text{density}
\item \theta \quad \text{polar angle}
\item \theta' \quad \text{angle from stagnation point}
\item \phi \quad \text{potential function}
\item \psi \quad \text{stream function}
\end{itemize}
Subscripts

\begin{itemize}
  \item $f$ \hspace{1em} fuel
  \item $o$ \hspace{1em} oxidant
  \item $w$ \hspace{1em} droplet surface
  \item $\infty$ \hspace{1em} free stream value
  \item $n$ \hspace{1em} normal to sphere surface
\end{itemize}
Figure 1. Geometry of the multisphere cylindrical cell.

Figure 2. Typical distribution of point sources within the droplets.
Figure 3. Non-uniform mesh used by Tal et al..

Figure 4. The mesh used by Chen and Tong.

Figure 5. The composite mesh used by Launder and Massey.
Figure 6. The embedded grid used in the present study.
Figure 7a. The computational plane for the entire embedded grid (Fig. 6).

Figure 7b. The computational plane for curvilinear mesh (meshed area).

Figure 7c. The computational plane for spherical mesh (meshed area).
Figure 8. Local Nusselt numbers for calculations carried out with a different number of point sources placed within the droplets.
Figure 9. Isotherm pattern for two droplets at L/R = 8 and Pe = 90.

Figure 10. Isotherm pattern for two droplets at L/R = 16 and Pe = 90.
Figure 11. Local Nusselt number as a function of angle from the front stagnation point with Peclet number as a parameter and L/R = 16: a. upstream droplet; b. downstream droplet.
Figure 12. Local Nusselt number as a function of angle from the front stagnation point with Peclet number as a parameter and $L/R = 8$: a. upstream droplet; b. downstream droplet.
Figure 13. Local Nusselt number as a function of angle from the front stagnation point with Peclet number as a parameter and $L/R = 4$: a. upstream droplet; b. downstream droplet.
Figure 14. Overall average Nusselt number as a function of Peclet number with L/R = 16.

Figure 15. Overall average Nusselt number as a function of Peclet number with L/R = 8.
Figure 16. Overall average Nusselt number as a function of Peclet number with L/R = 4
Figure 17. Local Nusselt numbers for a linear array of six droplets with a Peclet number of 120. Note that beyond the sixth droplet in the array, the local Nusselt (and thus the overall average Nusselt number) will be essentially constant.

Figure 18. Comparison of local Nusselt numbers for two pairs of droplets, one pair with equal sizes, the other pair with the upstream droplet diameter 80% of the downstream droplet diameter.
Chapter 5

The Combustion of Linear Droplet Arrays in a Low Reynolds Number Viscous Flow

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The Combustion of Linear Droplet Arrays in a Low Reynolds Number Viscous Flow

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Introduction

Inter-droplet and inter-particle interactions are important phenomena in reactive flows, and the need for an improved understanding of such phenomena for the design of spray combustors and furnaces can hardly be over emphasized. Such interactions manifest in the form of an alteration of flow field, competition for the oxidizer and a varying fuel vapor concentration around individual droplets. The difficulties of modelling transport processes around a large number of droplets placed in arbitrary spatial fields is obvious. It is therefore necessary to study the combustion of only a limited number of droplets in simple geometries.

The aim of this study is to model the combustion of droplets in a one dimensional linear array, coaxial with the flow direction, at low Reynolds numbers, and provide comprehensive information on the flame structure and temperature and fuel vapor distributions around individual droplets. This study supplements the work of the authors [1,2] carried out for flow around linear arrays at intermediate and high Reynolds numbers. Even though, a linear array is not equivalent to a spray, such a simplification is important in understanding inter-droplet interactions and obtaining asymptotic results as the number of droplets increases. It is the asymptotic behavior that better approximates the combustion of droplets in a spray cloud.

In the past, extensive work has been done in modelling isolated burning droplets, but not much literature is available for the combustion of multi-droplet systems. In polydispersed sprays, small droplets (20 µm-80 µm) possess little inertia and therefore conform to the local flow structure. For such droplets, Reynolds numbers are of the O(0), and literature reviews [3,4,5] suggest the use of the classical, spherically-symmetric, analysis pioneered by Spalding [6]. This classical model is based on diffusive transport around a single droplet immersed in an infinite medium. Although this model is adequate to describe transport processes in sprays with large droplet spacings, it breaks down for dense spray clouds. Musarra et al. [7] have studied a volatilizing coal particle in a creeping flow. The calculation domain used was twenty times the diameter of the particle. Here again the results would differ if interactions were taken into account.

Aminzadeh et al. [8] have accounted for interactions between two dissolving spheres at low Reynolds and high Peclet numbers. Chen and Pfeffer [9] have extended the work by including a first order reaction in the fluid phase. An analytical solution for creeping flow in bipolar coordinates, and finite difference solutions for the transport equations were used to calculate local Sherwood numbers for the two spheres. It is interesting to note that Sherwood numbers were shown to be less than 2 for certain cases thereby highlighting the importance of interactions. Tal et al. [10] studied heat transfer around a pair of spheres for high Reynolds numbers and showed the difference in transport processes for an isolated sphere and interacting spheres. Although these papers do underscore the importance of interactions, their work cannot be extended
to more than two droplets. In the present model there is no such limitation. The Stokes solution has been extended for an nth ordered array of spheres [11] and is used to obtain the flow field. Such an approach has obvious computational advantages over models developed in [1,2] when applied for low Reynolds flows.

Mathematical Model

Consider the motion of small fuel droplets (20 μm-80 μm) in a surrounding fluid phase. The small size of the droplets allows them to flow with the gas such that there is only a small relative velocity between the two phases. The Reynolds numbers based on relative velocity are small (Re<1) and the creeping flow solution may be used. Geometrical simplification is introduced by assuming the droplets to be equally spaced and in a linear array. The physical properties are assumed to be constant at the mean temperature of the gas. Internal circulation is neglected. The temperature of the droplets is fixed at the boiling point of the fuel. The Lewis number is set equal to one and the flame sheet approximation is assumed.

1. The solution procedure for the flow field:

To calculate the flow field, the Stokes solution for a single sphere is extended to a multi-droplet system. The general form of the solution for a single droplet in terms of stream function may be written as

\[ \nabla^2 (\nabla^2 \psi) = 0 \quad (1) \]

\[ \nabla^2 \psi = 2\omega \quad (2) \]

where

\begin{align*}
\nabla^2 & : \text{Stokesian operator} \\
\omega & : \text{vorticity}
\end{align*}

By superimposition with the free stream velocity \( U \), the general solution in terms of the stream function for flow past a single sphere is

\[ \psi = \frac{1}{2} U r_0^2 \sin^2 \theta_0 + \sum_{n=0}^{\infty} \left[ B_n r^{n+1} + D_n r^{n+3} \right] I_n(\xi) \quad (3) \]

Since (1) and (2) are linear, flow past \( N \) spheres from superimposition may be written as [11]:

\[ \psi = \frac{1}{2} U r_0^2 \sin^2 \theta_0 + \sum_{j=1}^{N} \sum_{n=0}^{\infty} \left[ B_{nj} r_j^{n+1} + D_{nj} r_j^{n+3} \right] I_n(\xi_j) \quad (4) \]
where the $I_n(\xi)$ is the nth order Gegenbauer polynomial, \(\xi = \cos \theta\), \(r^2 = x^2 + y^2\), and \((1/2)Ur_2\sin^2 \theta_0\) is the stream function for the uniform flow. As \(r \to \infty\), \(\Psi\) approaches the stream function of the uniform stream. Hence the boundary condition in the region far away from the droplets is satisfied identically. On the droplet surface, we have

\[
k(\frac{\partial \Psi}{\partial n})_o = \rho U_n L_v
\]

(5)

\[U_o = 0
\]

(6)

where \(L_v\) is the heat of vaporization, \(k\) is thermal conductivity of the gas; and \(U_n\) and \(U_o\) are the normal and tangential velocities respectively. By truncating Eqn. 4 and satisfying Eqns. 5 and 6 at M discrete points on the surface of each of the N droplets, we get \(2xMxN\) linear equations with that many unknowns. Solving for the unknowns, \(B_n\) and \(D_n\), the flow field is determined.

2. The solution procedure for the energy and species equations:

The linear droplet array in the present analysis is confined to a cylindrical cell [1]. The equations for conservation of energy and species for the axisymmetric flow in cylindrical coordinates, after using the Schvab-Zeldovich transformation are [12]:

\[
\beta_1 = \frac{C_p(T - T_m)}{L_v} + \frac{(Y_o - Y_{o_m})Q}{M_v \nu_0 L_v}
\]

(7)

\[
\beta_2 = \frac{Y_p Q}{M_p \nu_0 L_v} + \frac{(Y_o - Y_{o_m})Q}{M_v \nu_0 L_v}
\]

(8)

with the coupling functions defined as:

\[
\frac{\partial}{\partial x}(\gamma \nu C_p \beta_1) + \frac{\partial}{\partial y}(\gamma \nu C_p \beta_1) = \left[ \frac{\partial}{\partial x}(\nu \beta_1) + \frac{\partial}{\partial y}(\nu \beta_1) \right]
\]

(9)

\[
\frac{\partial}{\partial x}(\gamma \nu \beta_2) + \frac{\partial}{\partial y}(\gamma \nu \beta_2) = \left[ \frac{\partial}{\partial x}(\gamma \nu D \beta_2) + \frac{\partial}{\partial y}(\gamma \nu D \beta_2) \right]
\]

(10)

Once the flow field is obtained, the governing equation can then be solved numerically in an embedded grid [1]. The embedded grid consists of a spherical grid around every droplet and a curvilinear grid that covers the rest of the flow region. The spherical grid is used to provide an easy and accurate evaluation of temperature and concentration gradient around the droplet surface while the curvilinear grid is used to overcome the geometric complexities of the multiple droplet system. The governing equations are
transformed to generalized coordinates and solved by the numerical scheme SIMPLEM (Semi-Implicit Pressure Link Equation-Modified) [13]. It should be mentioned that since the present calculation does not involve solving any pressure-linked momentum equations, only the energy equation or species equation solver in the numerical scheme has been used during our calculation.

The boundary conditions for the temperature and species concentrations at the inlet and the boundary envelop are specified for the approach flow. At the axis of symmetry, symmetry conditions are applied. At the outlet, the flow properties are assumed to have zero gradients. The boundary conditions at the droplet surfaces are the energy-mass balance, and the mass balance for each species [12]. A guessed value for $\beta_1$ or $\beta_2$ is first assigned to every node in the entire domain and the calculations in these two domains are carried out, in turn, at each iteration to obtain an improved solution. Specifically, the curvilinear grid is calculated first and then the spherical grid. The new value of $\beta$ is then used in Eqn. 5 to improve the flow field. The entire iterative procedure is repeated until a converged solution is achieved.

Results and Discussion

In order to check the present numerical model, calculations were first carried out for isothermal mass transfer, without combustion, around a pair of spheres at different spacings, for small Reynolds numbers but large Peclet numbers. This case has also been studied by Aminzadeh et al. [7]. The average Sherwood numbers so obtained are plotted in Figs. 1a and 1b. As can be seen the agreement between the results of these two studies is good, therefore the present model can be extended for the study of combustion of multi droplet systems.

Results obtained for the combustion of a linear array with three droplets at two different Reynolds numbers and two different spacings are presented in Figs. 2 to 10. It must be pointed out that even though the creeping flow solution does not hold for $Re=1$ (inertial terms in the Navier Stoke's equation are of the same order as the viscous terms) it does provide an approximation to the flow field. Since particle interactions are stronger at higher Reynolds numbers [2], the approximate solution does provide a conservative estimate of the interactions.

Figs. 2 and 3 show the temperature distribution and fuel mass fraction around the droplets at $Re=0.1$ for two different spacings. Figs. 4 and 5 show the local Nusselt number plotted for the two cases. The isotherm for $T=1700 \, K$ represents the flame sheet. Notice that the flame sheet envelopes both the droplets irrespective of the spacing. The burning rate, which is proportional to the Nusselt number for this model, can be directly derived from Figs. 4 and 5. For the larger spacing, the local Nusselt numbers for the three spheres are quite similar and nearly constant along the surface of the droplets. The constant Nusselt numbers are to be expected, as the flow is completely symmetrical and diffusive transport is dominant. The similarity in the curves proves that there is very little or no interaction between droplets and each, therefore, burns independent of the other. However, the scenario changes for the smaller spacing. The heat and mass transfer at the front hemisphere of the leading droplet and the rear hemisphere of the third droplet does not change because those regions always in contact with cold gas, poor in fuel vapor. But in the inter-droplet spacing between these droplets, the gas is rich in fuel vapor, see Fig. 3b. This results in a decrease in temperature and concentration gradients leading to a decrease in heat and mass transfer. The burning rates of droplets therefore decrease as compared
to droplets at large spacings. Figs. 6 and 7 are the local Nusselt number of a linear array with four droplets at the same spacing and Reynolds number. In this figure, some periodic behavior in the burning rate of the second and third droplets can be observed and this periodic behavior could be a good approximation of typical droplet burning behavior in a spray.

The results for the higher Reynolds number, Figs. 8 to 10, are quite similar to the ones obtained before. The interactions are negligible for the large spacing but are appreciable for the smaller spacing. The only difference in these results is that the local Nusselt numbers are higher.
References


Figure 1a. Overall Sherwood number as a function of Peclet number with L/D=10.

Figure 1b. Overall Sherwood number as a function of Peclet number with L/D=4.
Figure 2a. Isotherms in the gas phase for three droplets burning at Reynolds number of 0.1 and spacing of 6 diameters.
Figure 2b. Fuel mass fraction in the gas phase three droplets burning at Reynolds number of 0.1 and spacing of 6 diameters.
Figure 3a. Isotherms in the gas phase for three droplets burning at Reynolds number of 0.1 and spacing of 2 diameters.

Figure 3b. Fuel mass fraction in the gas phase for three droplets burning at Reynolds number of 0.1 and spacing of 2 diameters.
Figure 4. Local Nusselt number vs angle from the front stagnation point at Re=0.1 and L/D=6.0.

Figure 5. Local Nusselt number vs angle from the front stagnation point at Re=0.1 and L/D=2.0.
Figure 6a. Isotherms in the gas phase for four droplets burning at Reynolds number of 0.1 and spacing of 2 diameters.
Figure 6b. Fuel mass fraction in the gas phase for four droplets burning at Reynolds number of 0.1 and spacing of 2 diameters.
Figure 7. Local Nusselt number vs angle from the front stagnation point at Re=0.1 and L/D=2.0.
Figure 8a. Isotherms in the gas phase for three droplets burning at Reynolds number of 1.0 and spacing of 6 diameters.

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Figure 11. Local Nusselt number vs angle from the front stagnation point at Re=1.0 and L/D=2.0.
Chapter 6

The Application of an Embedded Grid to the Solution of Heat and Momentum Transfer for Spheres in a Linear Array

Abstract

The objective of this study is to predict the forced convection heat transfer for spheres in a one-dimensional array aligned along the flow direction. An array with spheres of different sizes has also been studied. The interaction among these spheres is a salient feature of the analysis. The Navier-Stokes equations, in pressure-velocity form, and the energy equation have been solved numerically by an iterative finite-difference method in an embedded, body-fitted grid. A range of Reynolds numbers from 5 to 100 has been investigated for two sphere spacings. The temperature distribution around the sphere array, as well as the drag coefficient and Nusselt number around the sphere surfaces have been calculated. The results show good agreement with the numerical and experimental results in the literature.
Introduction

Fuel droplet combustion has received considerable attention in recent years. Most theoretical work has focused on the combustion of a single, isolated droplet or on the group combustion behavior of sprays. It has been recognized, however, that in any spray combustion process, droplet-droplet interactions reduce the gasification rate of participating droplets. Hence it is necessary to gain a better understanding of these phenomena to improve our ability to predict the combustion behavior of fuel sprays.

A few theoretical approaches, based on an assumption of potential flow, have been proposed to model interacting droplet arrays. For two-droplet systems, bipolar coordinates were used by Umemura [1] to describe the interaction between droplet pairs. For various multi-droplet arrays, Labowsky [2] proposed a technique, based on method of images, to calculate the burning rate of each individual droplet in an array. All of the above calculations were performed for droplet arrays burning in a quiescent, oxidizing atmosphere, i.e. for diffusion controlled transfer processes.

In a real combustor, however, forced convection may dominate the transfer processes, and combustion conditions may differ considerably from those in a quiescent environment. Thus a diffusion-limited analysis is inadequate and the convective effects need to be taken into account. In particular, the effect of forced convection on droplet-droplet interactions depends both on the relative arrangement of spheres in an array and on the orientation of the array with respect to the flow direction.

Shuen [3] studied the combustion of a planar droplet array oriented normal to the approaching flow and concluded that the interaction decreases as the Reynolds number increases. In contrast, for arrays with droplets aligned in tandem along the flow direction, Aminzadeh et al.[4], Chen et al.[5], and Tal et al.[6,7] found that the interaction increases as the Peclet number or Reynolds number increases.

The linear droplet array, although an approximation of a dense spray system, provides a convenient system for the study of some key factors dominating the spray combustion process, such as the effects of Reynolds number, droplet-droplet spacing, and droplet size on the heat and mass transfer behavior of the participant droplets. In contrast to the single droplet case, which provides an upper limit for convective heat and mass transfer rates in the absence of droplet-droplet interactions, a linear array of droplets aligned with the flow allows for a maximum interaction between droplets. Thus the asymptotic behavior observed for downstream droplets will provide a corresponding lower limit for the heat and mass transfer rates. The behavior for droplets in a real, dense spray should fall between these two limits. An appreciation of this lower limit will allow improved, conservative engineering models of the complex spray process to be developed.

Another important characteristic of real sprays is the droplet size distribution. Clearly, the interaction between two or more droplets of different sizes needs to be described. The size differences, however, are neglected in most existing theoretical models because of the increased geometric complexity. Umemura [1] studied the combustion of pairs of droplets of different sizes in a quiescent environment and
concluded that, for any separation of the two droplets, the smaller droplet is affected by the interaction to a greater degree than the larger droplet.

In the present analysis, one dimensional sphere arrays similar to those treated by Chen [5] and Tal [6] are studied with the intention of providing additional insight into the spray combustion process. In order to isolate the effect of inter-sphere spacing on the sphere-sphere interaction, the spheres are equally spaced although this restriction can be easily relaxed in the present computational scheme. Furthermore, since the analysis is formulated as a pseudo-steady process, the temporal variation of droplet spacing, owing to non-uniform droplet drag, is not taken into account.

A multisphere cylindrical cell, as shown in Figure 1, is used for the calculation domain, and an embedded grid, as shown in Figure 2, fills the interior of the cell. The embedded grid used here eliminates both an inaccuracy and numerical complications introduced by the grid used by Tal [6] and Chen [5]. For example, around the sphere surface, an spherical grid is used in the embedded grid and the size of the grid around the sphere surface can be adjusted to very fine degree without increasing the number of the nodes. This not only can provide more accurate evaluation of the Nusselt number on the sphere surface, but also helps to resolve any steep temperature gradients occurring in the vicinity of the droplet surface; this feature is especially attractive in droplet combustion studies. Another advantage, although not so obvious in this analysis, is important in the study of transient droplet evaporation, where the droplet shrinks as time progresses. At each time step, the entire domain used in Ref. 5 and 6 needs to be regridded. In the embedded grid used here however, only the spherical grid needs to be regrided, and this is indeed relatively easier and more economical.

The Navier-Stokes equations and the energy equation are solved numerically by an iterative, finite-difference method. To better simulate the flow around spheres, variable gas properties are also included in the analysis. Numerical results are obtained for Reynolds numbers from 5 to 100 and two sphere spacings, 4 and 8 sphere radii, respectively. While there is no theoretical limit to the number of tandem spheres that can be included in this model, our present constraints of computer time and storage have precluded the study of more than three spheres.

Mathematical Formulation

The linear sphere array in the present analysis is confined in a multisphere cylindrical cell, as shown in Figure 1. For axisymmetric flow, the conservation equations for mass, momentum, and energy in cylindrical coordinates reduce to:

The continuity equation

\[ \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0 \]  \hspace{1cm} (1)
The momentum equations:

\( x - \text{component} \)

\[
\frac{\partial}{\partial x} (\rho u^2) + \frac{\partial}{\partial y} (\rho uv) = -\frac{\partial p}{\partial x} + \frac{2}{Re} \left[ y \frac{\partial \tau_{xx}}{\partial x} + (y \tau_{xy}) \right] + \frac{\partial}{\partial y} \frac{\partial p}{\partial y} + \frac{2}{Re} \left[ y \frac{\partial \tau_{yy}}{\partial x} + (y \tau_{yx}) \right] - \rho g \frac{\partial}{\partial y}
\]

\( y - \text{component} \)

\[
\frac{\partial}{\partial x} (\rho uv) + \frac{\partial}{\partial y} (\rho v^2) = -\frac{\partial p}{\partial y} + \frac{2}{Re} \left[ y \frac{\partial \tau_{xx}}{\partial y} + (y \tau_{yx}) \right] + \frac{\partial}{\partial y} \frac{\partial p}{\partial x} + \frac{2}{Re} \left[ y \frac{\partial \tau_{yy}}{\partial y} + (y \tau_{xy}) \right] - \rho g \frac{\partial}{\partial x}
\]

where

\[
\tau_{xx} = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \left[ \frac{1}{y} \frac{\partial (yv)}{\partial y} + \frac{\partial u}{\partial x} \right]
\]

\[
\tau_{xy} = \tau_{yx} = \mu \left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right]
\]

\[
\tau_{yy} = 2\mu \frac{v}{y} - \frac{2}{3} \mu \left[ \frac{1}{y} \frac{\partial (yv)}{\partial y} + \frac{\partial u}{\partial x} \right]
\]

The energy equation:

Neglecting the compression work and viscous dissipation, the energy equation can be written as:

\[
\frac{\partial}{\partial x} (\rho u h) + \frac{\partial}{\partial y} (\rho v h) = \frac{2}{P_c} \left[ \frac{\partial}{\partial x} (y k \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (y k \frac{\partial T}{\partial y}) \right]
\]

With constant heat capacity, the enthalpy \( h \) is related to temperature \( T \) as \( h = C_p T \) and the energy equation can be rewritten as

\[
\frac{\partial}{\partial x} (\rho u T) + \frac{\partial}{\partial y} (\rho v T) = \frac{2}{P_c} \left[ \frac{\partial}{\partial x} (y k \frac{\partial T}{C_p \partial x}) + \frac{\partial}{\partial y} (y k \frac{\partial T}{C_p \partial y}) \right]
\]

The following dimensionless variables have been used for above equations:
The boundary conditions for multisphere cylindrical cell are:

a. at the inlet
u = 1
v = 0
T = 1

b. on the cylindrical envelope
\frac{\partial u}{\partial y} = 0, u = 0
v = 0
T = T_i

c. on the sphere surface

v = 0
T = T_i

d. along the axis of symmetry
\frac{\partial T}{\partial y} = 0
\frac{\partial T}{\partial x} = 0

e. at the outlet
u is adjusted to satisfy global mass conservation relation
\text{see Appendix)
\( \tau_{r0} = \mu \left( \frac{\partial v_r}{\partial r} + \frac{v_r}{r} \frac{\partial}{\partial \theta} \right) \)  

(13)

\[ \tau_r = 2\mu \frac{\partial v_r}{\partial r} - \frac{2}{3} \mu \left[ \frac{\partial (r^2 v_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial (v_\theta \sin \theta)}{\partial \theta} \right] \]  

(14)

\[
v_r = u \cos \theta + v \sin \theta
\]

(15)

\[
v_\theta = u \sin \theta + v \cos \theta
\]

(16)

\[ C_{dp} = 2 \int_0^\pi p_r \sin 2 \theta d\theta \]  

(17)

The total drag is then

\[ C_d = C_{dp} + C_{dp'} \]  

(18)

In order to compare the present results with previously published data, a modified set of dimensionless groups, in which the fluid properties are evaluated at the film temperature, are defined as:

\[ Nu_f = 2R'(k_d^' / l_f^') (\partial T'/\partial r')_{s}(T_*' - T_z') \]  

(19)

\[ Re_f = 2R' u_\infty^' \rho_\infty^' / \mu_f^' \]  

(20)

\[ Pr_f = C_p \mu_f^' / k_f^' \]  

(21)
where the subscript f refers to the film temperature defined as
\[
T_f = \frac{\left( T' + T'' \right)}{2}
\]  
(22)

**Transformation of the Basic Equations:**

The set of conservation equations can be written in a more general form for a general dependent variable \( \phi \) as
\[
\frac{\partial}{\partial x} (\gamma \rho u \phi) + \frac{\partial}{\partial y} (\gamma \rho v \phi) = \frac{\partial}{\partial x} (\Gamma_y \frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y} (\Gamma_y \frac{\partial \phi}{\partial y}) + S_y
\]  
(23)

For the axial velocity component (\( u \)) in the momentum equation
\[
\phi = u, \quad \Gamma = \frac{2\mu}{Re}, \quad \text{and} \quad S = -\frac{\partial p}{\partial x} + \text{viscous terms}
\]  
(24)

for the radial velocity component (\( v \))
\[
\phi = v, \quad \Gamma = \frac{2\mu}{Re}, \quad \text{and} \quad S = -\frac{\partial p}{\partial y} + \text{viscous terms}
\]  
(25)

and for the energy equation
\[
\phi = T, \quad \Gamma = \frac{2k}{PecP}, \quad \text{and} \quad S = 0
\]  
(26)

When new independent variables \( \xi \) and \( \eta \) are introduced, the partial derivatives of the function \( \phi \) are transformed according to
\[
\phi_x = (y_\eta \phi_\xi - x_\xi \phi_\eta) / J \quad \phi_y = (-x_\xi \phi_\eta + x_\xi \phi_\eta) / J
\]  
(27)

where \( J \) is the Jacobian of the transformation given by \( J = x_\xi y_\eta - x_\eta y_\xi \). By defining the following functions:
\[
G_1 = u y_\eta - v x_\eta
\]  
(28.a)
\[
G_2 = v x_\xi - u y_\xi
\]  
(28.b)
\[
\alpha = x_\eta^2 + y_\eta^2, \quad \beta = x_\xi x_\eta + y_\xi y_\eta, \quad \gamma = x_\xi^2 + y_\xi^2
\]  
(29)

one can reduce (23) to
\[
\frac{2}{\partial \xi} (\rho y G_1 \phi) + \frac{2}{\partial \eta} (\rho y G_2 \phi) = \frac{2}{\partial \xi} [(\gamma y/J)(\alpha \phi_z - \beta \phi_\eta)] + \frac{2}{\partial \eta} [(\gamma y/J)(\gamma \phi_\eta - \beta \phi_z)] + SyJ \tag{30}
\]

Integration over the control volume and application of Green's theorem allows equation (30) to be written in integral form as:

\[
\int_B (\rho y G_1 \phi \partial \eta - \rho y G_2 \phi \partial \xi) = \int_B [(\gamma y/J)(\alpha \phi_z - \beta \phi_\eta) \partial \eta + (\gamma y/J)(\gamma \phi_\eta - \beta \phi_z) \partial \xi + (\gamma y/J) d\xi \partial \eta] + \int_R SyJ d\xi \partial \eta \tag{31}
\]

With the notation shown in Figure 3 for a typical grid node P enclosed in its cell and surround by its neighboring nodes N, S, E, and W, the finite difference approximation of equation (31) over the cell can be written as

\[
(\rho y G_1 \phi \Delta \eta \Delta \xi) = [(\gamma y/J)(\alpha \phi_z - \beta \phi_\eta) \Delta \eta \Delta \xi + (\gamma y/J)(\gamma \phi_\eta - \beta \phi_z) \Delta \xi \Delta \eta] + SyJ \Delta \xi \Delta \eta \tag{32}
\]

If the power law scheme [8] is used to evaluate the strength of convection and diffusion on the cell boundary, equation (32) can be recast as a relation between the value of \( \phi \) at node P and its values at the neighboring nodes, i.e.

\[
A_p \phi_p = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + SYJ \Delta \xi \Delta \eta - [(\gamma y/J) \beta \phi_\eta \Delta \eta \Delta \xi] + [(\gamma y/J) \beta \phi_z \Delta \xi \Delta \eta] \tag{33}
\]

where \( A_p = A_E + A_W + A_N + A_S \) and the coefficients \( A_i \) (i = E, W, N, S) involve the convective flow parameters such as mass fluxes, areas, viscosities, diffusion coefficients, and the like. The details can be found in Reference [8]. The terms within the bracket in equation (33) result from the non-orthogonal grid system. They can be evaluated through the finite difference approximation

\[
[(\gamma y/J) \beta \phi_\eta \Delta \eta \Delta \xi] = \frac{1}{4} [(\gamma y/J) \beta \Delta \eta \Delta \xi] (\phi_{NE} - \phi_{SE} + \phi_{N} - \phi_{S}) \tag{34}
\]

**Pressure Equation**

In the momentum equations, the pressure remains unknown. However, an independent equation for pressure can be set up by combining the continuity and momentum equations. The details of the procedure will be described later in this section.

The disadvantage of using the pressure/velocity formulation, as compared to the stream function/vorticity formulation, is that checkerboard pressure and velocity fields may result [8]. Such unrealistic fields are linked to the use of central difference equations to express the first order derivatives of pressure in the momentum equations and velocity in the continuity equation. The most common way to avoid these
checkerboard fields is to use a staggered grid [8]. For a curvilinear grid, however, a staggered grid can be overwhelmingly complicated.

There are a number of numerical schemes available, such as SIMPLE (Semi Implicit Method for Pressure Linked Equations [9]), SIMPLER (SIMPLE-Revised [10]), or SIMPLEM (SIMPLE-Modified [10]), that can be used to solve the equations for pressure and momentum. These numerical schemes can avoid checkerboard pressure and velocity fields without adopting a staggered grid. In the present analysis, SIMPLEM is adopted because of its good convergence characteristics, and the pressure equation is formulated accordingly. The procedure and the strategy of SIMPLEM will be discussed briefly in the next section. The pressure equation is derived by writing the momentum equations in the following form:

\[
\begin{align*}
\text{u} &= u^* + B_1(y \partial p/\partial \xi) + C_1(y \partial p/\partial \eta) \\
\text{v} &= v^* + B_2(y \partial p/\partial \xi) + C_2(y \partial p/\partial \eta)
\end{align*}
\] (35)

where

\[
\begin{align*}
u^* &= \sum_{\text{EWNS}} A_i^\nu + S^\nu \text{ (37a)} \\
u^* &= \sum_{\text{EWNS}} A_i^\nu + S^\nu \text{ (37b)} \\
B_1 &= -y_\eta \Delta \xi \Delta \eta/A_p^\nu \text{ (37c)} \\
C_1 &= y_\xi \Delta \xi \Delta \eta/A_p^\nu \text{ (37d)} \\
B_2 &= x_\eta \Delta \xi \Delta \eta/A_p^\nu \text{ (37e)} \\
C_2 &= -x_\xi \Delta \xi \Delta \eta/A_p^\nu \text{ (37f)} \\
A_i^\nu &= A_i^\nu/A_p^\nu \text{ (37g)} \\
A_i^\nu &= A_i^\nu/A_p^\nu \quad i=E,W,N,S \text{ (37h)}
\end{align*}
\]

and \(S^u\) and \(S^v\) are residues after the pressure gradient terms have been extracted.

Integration of the continuity equation (equation 1) over the control volume yields

\[
(p G_1 y \Delta \eta)_x - (p G_1 y \Delta \eta)_w + (p G_2 y \Delta \xi)_x - (p G_2 y \Delta \xi)_w = 0
\] (38)

With the above definitions of \(u\) and \(v\), \(G_1\) and \(G_2\) can be written as follows:
\[ G_1 = G_1^* + (B_1 y_1 - B_2 x_1) (y \partial p / \partial \xi) + (C_1 y_1 - C_2 x_1) (y \partial p / \partial \eta) \quad (39.\text{a}) \]
\[ G_2 = G_2^* + (C_2 x_2 - C_1 y_2) (y \partial p / \partial \eta) + (B_2 x_2 - B_1 y_2) (y \partial p / \partial \xi) \quad (39.\text{b}) \]

where
\[ G_1^* = u^* y_1 - v^* x_1 \quad (40.\text{a}) \]
\[ G_2^* = v^* x_2 - u^* y_2 \quad (40.\text{b}) \]

With the substitution of \( G_1 \) and \( G_2 \) in the continuity equation (Equation 38), the pressure equation can be written as the algebraic equation:
\[ a_P p_P = a_P p_T + a_W p_W + a_N p_N + a_S p_S + b \quad (41) \]

where
\[ a_P = a_P + a_N + a_W + a_S \quad (42a) \]
\[ a_E = - (py^2 B) \eta (\Delta \xi / \partial \xi) \quad (42b) \]
\[ a_N = - (py^2 C) \eta (\Delta \xi / \partial \eta) \quad (42c) \]
\[ a_S = - (py^2 C) \delta (\Delta \xi / \partial \xi) \quad (42d) \]
\[ B = B_1 \partial y / \partial \eta - B_2 \partial x / \partial \eta \quad (42e) \]
\[ C = C_2 \partial x / \partial \xi - C_1 \partial y / \partial \xi \quad (42f) \]
\[ b = (p G_1^* y \Delta \eta)|_w - (p G_1^* y \Delta \eta)|_n + (p G_2^* y \Delta \xi)|_w - (p G_2^* y \Delta \xi)|_n + b_{no} \quad (42g) \]

In the above equation \( b_{no} \) is the contribution due to non-orthogonality. It is expressed as:
\[ b_{no} = [(C_1 y - C_2 x) (y^2 \partial p / \partial \eta)]_w - [(C_1 y - C_2 x) (y^2 \partial p / \partial \eta)]_n \]
\[ + [(B_2 x - B_1 y) (y^2 \partial p / \partial \xi)]_w - [(B_2 x - B_1 y) (y^2 \partial p / \partial \xi)]_n \quad (43) \]

**Solution Procedure**

The numerical scheme SIMPLEM was used to solve the momentum and continuity equations. The procedure of SIMPLEM, together with the solution procedure of solving the coupled energy equation, can be summarized as following:
Start with assumed values for the fields $u$, $v$, $P$ and $T$.

Calculate the coefficients of the momentum equations and the $u^*$ and $v^*$. Use these values to find $G_1^*$ and $G_2^*$ at grid nodes. Interpolate linearly to find $G_1^*$ and $G_2^*$ at the control volume faces.

Calculate the coefficients of the pressure equation and solve it to obtain a new pressure field.

Update $G_1$ and $G_2$ (Eq. 39) at the interfaces using the new pressure field, and using $1-\Delta \xi$ or $1-\Delta \eta$ centered difference scheme for $P$.

Use the updated $G_1$ and $G_2$ to recalculate the coefficients of momentum equation and use the new pressure field (obtained in step 2) to calculate the pressure gradient in the momentum equation with a $2-\Delta \xi$ or $2-\Delta \eta$ centered difference scheme. The momentum equation can then be solved to obtain a new velocity field, i.e. new $u$ and $v$.

With the new velocity field, calculate the coefficients of the energy equation and solve it to obtain a new temperature field.

Use the calculated $u$, $v$, $P$ and $T$ as new guess, return to step 2, and repeat until a converged solution is achieved.

The purpose of using a centered $1-\Delta \xi$ or $1-\Delta \eta$ pressure difference scheme in step 4 is to detect any oscillation occurring in the flow field, and to suppress it immediately with the interface velocity. The recalculation of the coefficients of the momentum equation in step 5, after updating the interface velocities, is to ensure that velocities used in the coefficients and the pressure field satisfy the same continuity equation. A more detailed discussion of the SIMPLEM procedures can be found in Reference [10]. A standard tri-diagonal matrix algorithm (TDMA) is used to solve for the pressure equation in step 2, the velocity equation in step 5, and the temperature equation in step 6. The details of TDMA can be found in Reference [8].

The Grid System

The grid system used for the present analysis, as shown in Figure 2, is an embedded grid. Close to the sphere, a spherical grid is retained. The remaining flow region is covered with a curvilinear mesh, which is generated by the method developed by Knight et al. [11]. This technique consists of solving Poisson's equation and performing an intermediate and final transformation. The generated grid can be either orthogonal (with partial control of the mesh spacing) or nearly orthogonal (with full control of mesh spacing.) In this work, we used the first of these options. Since orthogonality is not required for the curvilinear mesh, however, any other appropriate technique can be used to generate the mesh. With this embedded grid, the computational domain can then be as shown in Figure 4 (a). Figures 4(b) and 4(c) show the transformed calculation domain and the boundaries (meshed area) for the curvilinear mesh and spherical mesh, respectively. The calculations are carried out in each of the two domains at each iteration, first in the curvilinear mesh and then in the spherical mesh. It can be seen from Figure 4(b) that one row of the interior nodes in the spherical mesh serves as a boundary condition for the calculation in the curvilinear mesh. Figure 4(c) indicates how the intersection between the curvilinear mesh and the spherical mesh serves as a boundary condition when the calculation is performed in the spherical mesh. It should be mentioned that the slab corners in the transformed domain are points which require special treatment. In this study the values at the special points were obtained by linear interpolation between the neighboring
Nodes along the axis of symmetry in the physical domain; a linear distribution of partial derivatives in the
neighborhood of a special point was assumed. Other technique for treating the special point can be found
in Reference [12].

Results and Discussion

Calculations were first carried out for a single, isolated sphere immersed in flowing air. Experimental
and numerical data for this case are abundant [13]. For these calculations, all the data, as well as the
transport coefficients and thermodynamic properties are taken directly from the work of Renksizbulut and
Yuen [13] in order to compare the present results to their results. The sphere temperature, air temperature,
and Prandtl number (based on free stream properties) were taken as 353 °K, 800 °K, and 0.689, respectively.
The transport coefficients for air were approximated by \( \mu = T^{0.67} \) and \( k = T^{0.81} \). The air density varied with
temperature as \( \rho = 1/T \) and the heat capacity was taken as \( C_p = 1 \). The envelope of the multisphere cylindrical
cell was set at 12 radii away from the axis of symmetry to ensure zero gradients on the envelope. The inlet
and outlet of the cell were kept at a distance of about 8 radii from the spheres.

The criterion of convergence between two successive iterations was originally set at \( 10^4 \) in order
to conserve computer time. However, it was found that the resulting dependance of average Nusselt number
on Reynolds number was not smooth and tended to oscillate. This same phenomenon has also been reported
by Amizadeh [4]. Therefore, a criterion of convergence of \( 10^5 \) was used and good results were obtained.
A relaxation factor of 0.8 was used for the calculation at Reynolds numbers below 50, while for Reynolds
numbers greater than 50, a relaxation factor of 0.6 was used.

The calculated drag coefficients and average Nusselt numbers of the isolated solid sphere are
compared with the numerical results of Renksizbulut and Yuen [13] in Figures 5 and 6. Note that here the
Reynolds number and the average Nusselt number are evaluated at the film temperature. The agreement
between the present results and the results of [13] is very good. Since the numerical results in Reference
[13] correlate with a wide range of experimental data, the present results are also in good agreement. This
favorable comparison validates the present analysis and the numerical procedure, and justifies extending
the calculations to a multisphere system. Numerical solution have been obtained for three-sphere arrays
with sphere spacings of 4 and 8 radii, and an array with spheres of three different sizes. The calculation were
performed in a mesh consisting of a 150 x 42 grid plus three spherical meshes with 21 x 11 grids (see Figure
2) and the CPU time requirement is typically about 30 min in a Floating Point System (FPS) 264 to reach
converged solutions for most cases discussed below. For a sphere array with spacing of 4 radii, the flow
field and the isotherm pattern at Re=100 can be seen in Figures 7(a), (b), (c), and Figure 8(a). In Figures 7(b)
and (c), it can be seen that the second and third sphere clearly interact with the wake of the first and second
sphere, respectively.

In Figure 8(a), very similar isotherm patterns can be observed among these three spheres, however,
these patterns are not periodic. Figure 8(b) shows the isotherms of the three-droplet array with spacing of
8 radii at Re=100. As can be seen in Figure 8(b), a periodic behavior emerges for the isotherm pattern of
second and third sphere. This periodic behavior was not observed in Tal's work [6], and the discrepancy
might owe to the shorter spacings (3 and 6 radii) used in their study. For comparison, the isotherms for the array with three different sizes of spheres at Re=50 are also presented here and shown in Figure 8(c).

Figures 9(a) and 9(b) show the local Nusselt number for each of three spheres with a spacing of 4 and 8 radii at Reynolds numbers of 100. It is interesting to note in Figure 9(a) that the wake behind the spheres at Re=100 tends to increase the Nusselt number in the region after the polar angle of 140 (measured from the front stagnation point). The local Nusselt numbers of the first sphere in the array is slightly greater than those for an isolated sphere in the same region. In Figure 9(b), however, the local Nusselt numbers around the first sphere are the same as that of a single, isolated sphere. This indicates the heat transfer of the first sphere is not influenced by the presence of the downstream spheres. Comparison of Figure 9(a) and Figure 9(b) shows that the local Nusselt numbers for the second and third spheres, at larger spacing, is higher than those for the same spheres at smaller spacing, which shows the sphere-sphere interaction decreases as the spacing between the spheres increases.

The result of overall average Nusselt number and total drag coefficient at sphere spacing of 4 and 8 radii as a function of Reynolds number are shown in Figures 10 and 11, respectively. These results confirm the local variations discussed above. Particularly, it can be observed that when the sphere spacing is increased, the difference of the average Nusselt number and the total drag coefficient between the first sphere and the rest of the spheres is reduced, i.e., the interaction is reduced. The value of the Nusselt number and total drag coefficient is higher for the first sphere, and the values for the second and the third sphere are nearly the same. This agrees with the results reported by Chen [5] and Tal [6].

The local Nusselt numbers for three spheres with different sizes and equal size at Re = 50 are shown in Figures 12 and 13 respectively. In Figure 12, radius of the largest sphere (third sphere) is used to be the characteristic length for the local Nusselt number and Reynolds number. It can be observed that the smallest sphere (first sphere) has the highest heat transfer rate on the sphere surface. Comparison between Figure 12 and Figure 13 indicates that the small upstream spheres give less influence on the heat transfer of the downstream spheres.

**Conclusions**

A numerical scheme, SIMPLEM, and an embedded, body fitted grid are used to obtain the solution of heat and momentum transfer in one-dimensional sphere arrays for Reynolds numbers from 5 to 100. The following conclusions can be drawn from this analysis:

1. The present numerical scheme has been applied to a single, isolated sphere and the results show good agreement with the available numerical results and experimental data.
2. The calculations in the present analysis are based on variable gas properties. Since most practical heat transfer problems involve large property variations, the present study appears to be more relevant than those where constant properties are assumed.
3. The interaction between equal-size spheres is found to decrease as the sphere spacing increased. For spheres with different sizes, it is also found that small sphere tends to have a higher heat transfer rate.
and less influence on the heat transfer of the downstream spheres.

4. The velocity-pressure form used for the momentum equation in the present study could be more easily extended to three dimensional problems than the stream-function/vorticity form used in most other related analyses reported in the literature.

5. For linear droplet arrays undergoing combustion, the present heat transfer analysis, when coupled with the species conservation equations, can be used to calculate the burning rate of linear droplet arrays. This analysis is currently undergoing and the results will be reported in future communications.

Acknowledgement

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References


Appendix

The velocity component $u$ at the outlet of the cylindrical cell is adjusted to satisfy mass conservation at each iteration as follows.

The total mass flow rate (based on unit radian) into the cylindrical cell is calculated at the cell inlet as

$$Q = \sum_{j=1}^{M} \rho \Delta Y_j Y_j u_j$$

An estimate of the total outlet flow is calculated using the $u$ component of velocity one node upstream of the exit as

$$Q = \sum_{j=1}^{M} \rho_j^{L-1} \Delta Y_j Y_j u_j^{L-1}$$

The $u$ component of velocity at the exit of the cylindrical cell is then adjusted by

$$u_j^{L-1} = u_j^{L-1} \left( \frac{Q}{Q} \right)$$

where $j$ is the index of the node in $y$ direction,

- $M$ is the largest number of $j$,
- $\Delta Y_j Y_j$ is the flow area associated with node $j$,
- $L$ is the index of outlet,
- $L-1$ is the index of the interior nodes one node upstream from the outlet, and
- $Q$ (or $Q$) is the actual (estimated) mass flow rate.
Nomenclature

A \hspace{1cm} \text{coefficient in the general finite difference equations}
C_d \hspace{1cm} \text{total drag coefficient}
C_{dr} \hspace{1cm} \text{friction drag coefficient}
C_{dp} \hspace{1cm} \text{pressure drag coefficient}
C_p \hspace{1cm} \text{heat capacity}
G \hspace{1cm} \text{convective term normal to grid cell boundary}
h \hspace{1cm} \text{nondimensional enthalpy}
J \hspace{1cm} \text{Jacobian of transformation}
k \hspace{1cm} \text{thermal conductivity}
L \hspace{1cm} \text{distance between the centers of two spheres}
Nu \hspace{1cm} \text{Nusselt number}
p \hspace{1cm} \text{nondimensional pressure}
Pe \hspace{1cm} \text{Peclet number}
Pr \hspace{1cm} \text{Prandtl number}
R \hspace{1cm} \text{radius of droplets}
Re \hspace{1cm} \text{Reynolds number}
S \hspace{1cm} \text{source term in the finite difference equation for general variables d}
T \hspace{1cm} \text{nondimensional temperature}
u, v \hspace{1cm} \text{nondimensional x and y component of velocities}
v_r, v_\theta \hspace{1cm} \text{nondimensional r and \theta component of velocities in spherical coordinate}
x, y \hspace{1cm} \text{axial and radial coordinates}

\begin{align*}
\alpha, \beta, \gamma & \hspace{1cm} \text{coordinate transformation parameter nondimensional natural coordinates} \\
\delta \xi, \delta \eta & \hspace{1cm} \text{finite difference mesh spacing in } \xi \text{ and } \eta \text{ direction in the transformed plane} \\
\Delta \xi, \Delta \eta & \hspace{1cm} \text{cell boundary sizes in } \xi \text{ and } \eta \text{ directions in the transformed plane} \\
\Gamma & \hspace{1cm} \text{effective diffusity for general variable d} \\
p & \hspace{1cm} \text{nondimensional density} \\
\mu & \hspace{1cm} \text{nondimensional viscosity} \\
\tau & \hspace{1cm} \text{surface shear stress} \\
\theta & \hspace{1cm} \text{angle from stagnation point} \\
\phi & \hspace{1cm} \text{general variable}
\end{align*}

Superscript

- \hspace{1cm} \text{averaged quantity}
' \hspace{1cm} \text{dimensional quality}
u \hspace{1cm} \text{u component}
v \hspace{1cm} \text{v component}
Subscript

\(e,w,n,s\) \hspace{0.5cm} \text{control volume faces surrounding point } p \\
\(E,W,N,S\) \hspace{0.5cm} \text{neighboring points surrounding point } p \\
f \hspace{0.5cm} \text{film condition} \\
r \hspace{0.5cm} \text{radial coordinate in spherical geometry} \\
s \hspace{0.5cm} \text{sphere surface} \\
\(\theta\) \hspace{0.5cm} \text{angular coordinate in spherical geometry} \\
\phi \hspace{0.5cm} \text{angle around the symmetric axis} \\
\(\infty\) \hspace{0.5cm} \text{free stream value}
Figure 1. Geometry of multisphere cylindrical cell.

Figure 2. Embedded grid for the present numerical study.
Figure 3a. Finite-difference grid representation in physical plane.

Figure 3b. Finite-difference grid representation in transformed plane.
Figure 4a. The computational plane for the entire embedded grid (Fig. 2).

Figure 4b. The computational plane for curvilinear mesh (meshed area).

Figure 4c. The computational plane for spherical mesh (meshed area).
Figure 5. Drag coefficient for an isolated solid sphere.

Figure 6. Numerical heat transfer data for an isolated solid sphere.
Figure 7a. Velocity field in the entire cylindrical cell for a three-sphere array at Re=100 and L/R=4.0.

Figure 7b. Velocity field around the first and the second spheres.

Figure 7c. Velocity field around the second and the third spheres.
Figure 8a. Isotherm pattern for three spheres at Re=100 and L/R=4.0.

Figure 8b. Isotherm pattern for three spheres at Re=100 and L/R=8.0.

Figure 8c. Isotherm pattern for three different-size spheres at Re=50 and L/R3=4.0.
Figure 9a. Local Nusselt number vs angle from the front stagnation point at Re=100 and L/R=4.0.

Figure 9b. Local Nusselt number vs angle from the front stagnation point at Re=100 and L/R=8.0.
Figure 10b. The average Nusselt number vs Reynolds number at L/R=8.0.
Figure 11a. Total drag coefficient vs Reynolds number at L/R=4.0.

Figure 11b. Total drag coefficient vs Reynolds number at L/R=8.0.
Figure 12. Local Nusselt number vs angle from the front stagnation point for three different-size spheres at Re=50 and L/R3=4.0.

Figure 13. Local Nusselt number vs angle from the front stagnation point for three equal-size spheres at Re=50 and L/R=4.0.
Chapter 7

The Combustion of Linear Droplet Arrays

Abstract

The goal of this work is to elucidate the details of two key factors dominating the droplet burning behavior in sprays: droplet-droplet interaction and convective flow. In order to make the problem manageable, a spray system with a simpler geometry and fewer droplets is desirable. Therefore, the combustion of a one-dimensional, linear droplet array in tandem with a convective flow has been studied. The governing transport equations were solved numerically in an embedded grid. A one-step, finite-rate kinetic model was employed to simulate the chemical reaction in the combustion process. Results for droplet arrays burning at two Reynolds numbers, 10 and 50, and two droplet spacings, 4 and 8 radii, were obtained. The results indicate that the droplet burning behavior is affected by Reynolds number, droplet-droplet spacing, and the relative location of droplets in the array. Therefore, the model for a single, isolated droplet is not adequate to represent typical droplet burning behavior in a spray. Droplet-droplet interaction was found to be stronger for arrays with smaller droplet spacing. For arrays with large droplet spacing burning at low Reynolds number, some asymptotic droplet burning behavior was observed.
Introduction

Droplet-droplet interactions are a common phenomena encountered during combustion of fuel sprays. Due to the great importance of fuel sprays in practical applications, it is essential that the droplet-droplet interactions be understood in order to enable a better design of fuel spray systems. Droplet-droplet interactions in a spray involve the interaction of the flow field around the participant droplets, the competition for oxidizer, mixing of fuel vapor, etc. Only a detailed study can describe such complex phenomena.

Although in the past few years Dwyer and Sanders\textsuperscript{1,2} have successfully described gaseous phase combustion for a single, burning fuel droplet in a convective flow, so far, except for the work of Sheun\textsuperscript{3} no detailed study for the combustion of multi-droplet systems has appeared in literature. However, Sheun's study only investigated the droplet burning behavior in a single layer of a planar droplet array normal to the flow. Hence a very important process in spray combustion, the interaction between the upstream droplet and downstream droplet, has been overlooked. Furthermore, the flame sheet assumption used in his study has proved to be quite inadequate in describing a typical droplet burning behavior.\textsuperscript{1,2}

Due to large number of droplets involved, the detailed study of a three dimensional spray system is infeasible for even the most sophisticated computer system. One way to overcome this problem is to study sprays with a simpler geometry and fewer droplets. Therefore, we have initiated our study with a simple spray system, a linear droplet array. Our intent is to gain some useful insight for the study of more complex spray combustion.

Mathematical Methods

Grid System

In order to facilitate numerical calculations, the droplet array was confined to a cylindrical cell.\textsuperscript{4} The transport equations were solved by a finite difference method in an embedded grid within the cylindrical cell (see Fig. 1). The embedded grid consists of spherical grids surrounding every droplet and a nearly orthogonal curvilinear grid covering the rest of the calculation domain. The curvilinear grid was generated by a numerical solution of Poission's equation.\textsuperscript{5}
Governing Equations

The dimensional governing equations may be written in the following forms:

The continuity equation

\[ \frac{\partial}{\partial x}(ypu) + \frac{\partial}{\partial y}(ypv) = 0 \]  

(1)

Momentum Equations

\textbf{x direction}

\[ \frac{\partial}{\partial x}(ypuu) + \frac{\partial}{\partial y}(ypuv) = -y^x + \frac{\partial}{\partial x} \left[ y \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial (y\tau_{xy})}{\partial y} \right] \]  

(2)

\textbf{y direction}

\[ \frac{\partial}{\partial x}(ypuv) + \frac{\partial}{\partial y}(ypvv) = -y^x + \frac{\partial}{\partial x} \left[ y \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial (y\tau_{yy})}{\partial y} \right] - \tau_{xy} \]  

(3)

where

\[ \tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \frac{2}{3} \mu \left[ \frac{1}{y} \frac{\partial (yy)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(4)

\[ \tau_{xy} = \tau_{yx} = \mu \left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right] \]  

(5)

\[ \tau_{yy} = 2\mu \frac{v}{y} \cdot \frac{2}{3} \mu \left[ \frac{1}{y} \frac{\partial (yy)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(6)

\[ \tau_{yy} = 2\mu \frac{\partial v}{\partial y} + \frac{2}{3} \mu \left[ \frac{1}{y} \frac{\partial (yy)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(7)
Energy Equation

\[
\frac{\partial}{\partial x} (ypuh) + \frac{\partial}{\partial y} (ypvh) = \left[ \frac{\partial}{\partial x} (yq_x) + \frac{\partial}{\partial y} (yq_y) \right]
\]

where

\[
h = \sum_{i=1}^{N} Y_i h_i , \quad h_j = \int_{r}^{r} C_{p,i} dT + \rho \sum_{i=1}^{N} \left( h_i D_i \frac{\partial Y_i}{\partial x} \right) , \quad q_x = -k \frac{\partial T}{\partial x} \cdot \rho \sum_{i=1}^{N} \left( h_i D_i \frac{\partial Y_i}{\partial y} \right)
\]

Species Conservation

\[
\frac{\partial}{\partial x} (ypuY_i) + \frac{\partial}{\partial y} (ypvY_i) = \left[ \frac{\partial}{\partial x} (ypD_i \frac{\partial Y_i}{\partial x}) + \frac{\partial}{\partial y} (ypD_i \frac{\partial Y_i}{\partial y}) \right] + \gamma c_i w_i
\]

Equation of state

\[
p = \rho RT \sum_{i=1}^{N} \left( Y_i / W_i \right)
\]

The following notation has been employed: \( \rho \) - density, \( u \) and \( v \) - velocity components, \( p \) - pressure, \( T \) - temperature, \( T_h \) - reference temperature, \( \tau \) - the Newtonian stress tensor, \( \mu \) - viscosity, \( k \) - thermal conductivity, \( D_i \) - binary diffusion coefficient, \( C_{p,i} \) - specific heats, \( h \) - enthalpy, \( h^o \) - heat of formation for species \( i \), \( w \) - consumption rate of the oxidized species in the reaction, \( Y_i \) - mass fraction of species \( i \), \( a_i \) - stoichiometric coefficient of species \( i \), \( W_i \) - molecular weight of species \( i \), \( N \) - total number of species, and \( R \) - the universal gas constant.

Boundary conditions

The boundary conditions for the velocity, temperature, and species concentrations at the inlet and the outer envelop are specified for the approaching flow. At the axis of symmetry, symmetry conditions are
applied. At the outlet, the velocity component v is set to be zero, velocity u adjusted to satisfy the global mass conservation relation, and the rest of the flow properties are extrapolated from the interior points. The boundary conditions of the droplet surfaces are the same as used in Ref. 6.

**Transport and Thermodynamic Properties**

Transport coefficients for viscosities and binary diffusion coefficients have been evaluated using the kinetic theory of Chapman and Enskog. The thermal conductivity of each constituent was calculated from the modified Eucken model. The thermal conductivity and viscosity of the mixture was calculated by the formulas recommended by Mathur, et. al. The heat capacities and the heat of formation were derived using JANAF polynomials.

**Numerical Scheme**

The momentum equations in this study, as shown in equations 2 and 3, are in pressure-velocity form. In the literature, a few numerical schemes such as SIMPLE (Semi Implicit Pressure Link Equation), SIMPLER (SIMPLE-Revised), and SIMPLEM (SIMPLE-Modified) are designed to solve the momentum equations in pressure-velocity form without adopting a staggered grid. In this work, we have used the numerical scheme SIMPLE. It should be mentioned that these numerical schemes were developed for a general coordinate system; therefore, the governing momentum, energy, and species equations were first transformed into the generalized coordinates and then solved in the transformed computational domain. The details of the transformation and the solution procedures of the numerical scheme can be found in Ref. 11.

**Results and Discussion**

In the present study, droplets are burning at same ambient flow conditions as those used by Dwyer and Sanders and the one-step global chemical reactions proposed by Westbrook, et al. are employed to simulate the chemical reaction in the gaseous flow field.

In order to reduce computational cost, we limited our computations to arrays with three droplets. The Reynolds number, ranging from 10 to 50 (based on the inflow properties), has been used to study the convective effect on the burning droplets. Also the droplet-droplet interactions at different droplet-droplet spacings can be revealed by arranging these three droplets at distances of 4 radii and 8 radii apart.
The computation has been performed for a single, isolated octane droplet at a Reynolds number of 67.8, a case that has been previously studied by Dwyer and Sanders. The results of the calculation are shown in Fig. 2. The agreement between these two studies is very good. Therefore, the present study can be extended to simulate multi-droplet systems.

Figures 3 and 4 show the combustion of droplet arrays with three methanol droplets at a Reynolds number of 10 and droplet spacings of 8 and 4 radii, respectively. It is interesting to note the difference in the flame structure in these two figures. Specifically, the flame sheath (i.e., the region between the two $T/T_e = 1.8$ isotherms) for larger droplet spacing (see Fig. 3) wraps each droplet individually, while for smaller spacing (see Fig. 4) the flame sheath covers the entire array just like it covers a single droplet. In order to better show the effect of droplet-droplet interaction on the burning rates of these two arrays, the local Nusselt numbers ($=2R_k \left( \frac{\partial T}{\partial r} \right)_f \left( T_{2} - T_e \right)$) around the droplets, as well as that of an isolated droplet, are shown in Figs. 5 and 6. In these two figures, the burning rates of the leading droplet are seen to be influenced very little by the presence of downstream droplets. However, in Fig. 5, where the droplet spacing is 8 radii, the burning rates around the second and the third droplet are higher than that of the corresponding droplets in Fig. 6, where the spacing is halved. This indicates that the droplet-droplet interaction, which usually reduces the burning rate of a droplet, has more impact on the downstream droplets and the interaction is stronger among the droplets with smaller spacing. This phenomena is a result of the convective flow, where the relatively cool, unburnt fuel vapor from the upstream droplets is carried into the inter-droplet region, reducing the temperature in that region, and, in turn, reducing the burning rate of the downstream droplets. For an array with smaller spacing, the shorter physical distance between droplets leads to less heating of the fuel vapor from the upstream droplets by the heat generated from the reaction zone before it reaches the vicinity of the downstream droplet. Thus the burning rate of the downstream droplets is more severely retarded. It should also be noticed that in Fig. 3 and Fig. 5, a great similarity of the isotherm patterns and local Nusselt number distributions arise around the second and third droplet. This similarity implies that an asymptotic behavior can be expected for droplets further downstream.

Figures 7(a,b) and 8(a,b) show the isotherms and fuel distributions for arrays burning at two different spacings and $Re=50$. For an array with larger droplet spacing (Figs. 7a and 7b), it can be seen that the isotherm pattern right behind the first droplet is unaffected and most of the fuel vapor around it is consumed. Furthermore, the temperature around the second and the third droplet (see Fig. 7a) is not reduced by the droplet-droplet interaction as would be expected, but is greatly increased in comparison with that of an isolated droplet. The significant increase in the temperature around the downstream droplet results from the increased burning in the inter-droplet region, caused by the abundant supply of the oxidizer. The combustion in the inter-droplet spacing consequently increases the temperature gradient and the burning rate around the downstream droplet. This can be more easily seen in Fig. 9, where the local burning rates of these three droplets are expressed in terms of local Nusselt numbers. For the array with smaller spacing (see Figs. 8a and 8b), however, due to the closeness of the second droplet, the reaction zone behind the
first droplet is almost squeezed out of its wake. It can also be observed (see Fig. 8a) that the second droplet, which happens to be located inside the flame zone of the first droplet, has a high temperature environment and, therefore, has a high burning rate. As for the third droplet in this array, with the significant amount of fuel vapor accumulating at the spacing between the second and the third droplets (see Fig. 8b), the burning rate around this droplet is severely reduced. This is clearly shown in Fig. 10.

The effect of convective flow on the burning rate of these arrays can be revealed by comparing Figs. 5 and 6 to Figs. 9 and 10. Enclosed by a continuous flame sheath, the leading droplet (or an isolated droplet) at Re=10 has a higher burning rate. For the downstream droplets, on the contrary, the droplets burning at Re=50 have higher burning rates because the flame sheath is blown closer to droplet surface by the stronger convective flow.

Conclusions

The pseudo steady-state combustion behavior of linear droplet arrays has been studied. The following conclusions are drawn from this work:

1. The droplet interaction, which usually reduces the burning rate of a droplet, is increased as the droplet-droplet spacing is decreased.

2. In the arrays studied, some asymptotic behavior is observed for the downstream droplets at large droplet spacing and low Reynolds number.

3. The burning behavior of a droplet in an array can vary significantly, depending on the Reynolds number, droplet location in the array, and the droplet-droplet spacing. Therefore, one should be wary when the results of an isolated burning droplet are used to represent the typical droplet burning behavior in a dense spray.

Acknowledgement

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References


Figure 1. The embedded grid for the present study.

Figure 2. Isotherms in the gas phase for a 88 μm octane droplet at Reynolds number of 67.8.
Figure 3. Isotherms in the gas phase for three 100 μm methanol droplets at Reynolds number of 10 and droplet spacing of 8 radii.
Figure 4. Isotherms in the gas phase for three 100 μm methanol droplets at Reynolds number of 10 and droplet spacing of 4 radii.
Figure 5. Local Nusselt number vs angle from the front stagnation point at Re=10 and L/R=8.0.

Figure 6. Local Nusselt number vs angle from the front stagnation point at Re=10 and L/R=4.0.
Figure 7a. Isotherms in the gas phase for three 100 μm methanol droplets at Reynolds number of 50 and droplet spacing of 8 radii.

Figure 7b. Fuel mass fraction contours in the gas phase for three 100 μm methanol droplets at Reynolds number of 50 and droplet spacing of 8 radii.
Figure 8a. Isotherms in the gas phase for three 100 μm methanol droplets at Reynolds number of 50 and droplet spacing of 4 radii.

Figure 8b. Fuel mass fraction contours in the gas phase for three 100 μm methanol droplets at Reynolds number of 50 and droplet spacing of 4 radii.
Figure 9. Local Nusselt number vs angle from the front stagnation point at Re=50 and L/R=8.0.

Figure 10. Local Nusselt number vs angle from the front stagnation point at Re=50 and L/R=4.0.
Chapter 8

Numerical Study of the Unsteady-State Combustion of A Linear Droplet Array

(to be submitted to Combustion Science and Technology)
NUMERICAL STUDY OF THE UNSTEADY-STATE COMBUSTION OF A LINEAR DROPLET ARRAY

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ABSTRACT

The detailed, time-varying combustion behavior of droplets in a linear array in parallel with a convective flow has been simulated numerically. An embedded grid is used to deal with the change of droplet size and spacing during the combustion process. A one-step, finite-rate kinetic model is employed to simulate the chemical reaction in the gaseous phase. The results from the present model for a single, isolated droplet agree well with the results reported by other investigators. The calculations for an array with three droplets indicate that, at the initiation of droplet burning, ignition occurs simultaneously behind each individual droplet, and a continuous, thick flame layer develops. Located inside the thick flame layer from the precedent droplet, the downstream droplet has a higher mass burning rate than the leading droplet. Owing to the difference in the drag forces, the droplet-spacing variation for the first two droplets is significant. However, the variation of spacing between the downstream droplets is negligible. For the time interval studied, the Nusselt number, velocity, size, and drag force for downstream droplets tend toward asymptotic values.
Introduction

Despite being commonly used in wide variety of applications, spray combustion, owing to its complexity, is not yet well understood. A typical spray combustion process usually involves the simultaneous evaporation of a large number of droplets, complex fluid mechanics around the droplets, rapid chemical reaction in the gaseous phase, and interaction among the droplets. The understanding of the detailed behavior of these processes is the key to the success of many group combustion model. However, to study, analytically or experimentally, the detailed behavior is not presently feasible, and thus there is a need to develop a reasonable numerical model to approximate these processes.

In the past few years, Dwyer and Sanders [1,2,3] have successfully developed a model to simulate the detailed burning behavior for a single, isolated droplet in a convective flow. In their work, they simulate the combustion of a droplet injected into a hot, convective environment. The results show that, as the droplet velocity is reduced by the drag force, the burning process of the droplet is transformed from one that is convection dominated to one controlled by conduction and diffusion. Also, by using global, finite-rate chemical kinetics to simulate the gas-phase combustion, they predict a thick flame sheath around the droplet. This discovery challenges the validity of the flame sheet assumption, an assumption commonly used in combustion studies. Although the model they proposed can describe well the detailed burning behavior of a single droplet, it is unrealistic when applied to the typical burning behavior of droplets in a dense spray. For in the combustion of a dense spray, droplets interact with their neighboring droplets, and the interactions among the droplets have a significant effect on droplet burning rate. In order to take into account the effect of droplet-droplet interactions, a study of arrays with multi-droplets is necessary. The detailed simulation of a three-dimensional array with a large number of droplets is beyond our current computational resources. The study of an one-dimensional linear droplet array with small number of droplets, however, can reveal many of the important aspects of a typical spray-combustion process.

Although studies on the convective heat transfer for spheres in a linear array have clearly demonstrated the significance of interactions between upstream and downstream spheres on heat transfer rates [4,5], the significance of interactions between evaporating or burning droplets in a convective flow has received little attention. Recently, Patnaik [6] developed a model to describe the life time history of two interacting droplets evaporating in a co-axial, convective environment. His results show that the upstream droplet has little effect on the flow pattern of the downstream droplet at the droplet spacing (8.5 radii) and Reynolds numbers (100 and 50) he chose. However, the burning rate of the downstream droplet is noticeably reduced, owing to the presence of upstream fuel vapor around the downstream droplet. Raju [7] carried out a similar computation for two interacting droplets. In his study, however, the droplet spacing was time dependent. The results indicate that, owing to the relative difference in the drag forces on the droplets, the droplet spacing is reduced from the original eleven to less than two droplet diameters by the time 10% of the droplet volume is evaporated. During this time period the interaction between vaporizing droplets is found to be significant, i.e., the evaporation rate (or Nusselt number) of the second droplet is severely reduced. Anticipating that a burning array might behave quite differently from an evaporating array, the
present authors proposed a steady-state model [8] to simulate the detailed burning behavior of a threedroplet linear array in which the combustion is described by the finite rate chemical kinetics used by Dwyer and Sanders. The results indicate that, at a low Reynolds number (Re=10), a continuous flame sheath covers the entire droplet array and the burning rate of the leading droplet is higher than that of the downstream droplets. At a higher Reynolds number (Re=50), the flame sheath is blown into the inter-droplet region causing a drastic increase in the burning rate for the downstream droplets. Calculations were also carried out for arrays with different spacings, and it was found that the effect of droplet interactions is increased as the droplet spacing is decreased. Through this study, the effects of convective flow and droplet spacing on the droplet burning rate were quantitatively demonstrated. However, owing to the steady-state assumption, the model is not adequate to describe a real burning linear array. For example, in the steady state model, the variation of droplet size and spacing is not considered. In any real situation, however, droplet size and spacing are varying with time because of mass loss through evaporation and differences in the drag forces on the droplet surfaces. The variation of droplet size, or the droplet spacing, alters the flow field and flame structure, which in turn, affects droplet burning rate. In order to describe the details of such a complex process, an unsteady-state model is clearly necessary.

In this work, we extend our previous steady-state model to simulate the time-varying combustion process of a linear array, co-axial in a hot, convective flow. The purpose of this study is to provide information on some of the key descriptive features of the process, such as Nusselt number, drag coefficient, and droplet size and velocity variations during the droplet history. Other interesting features, such as the transient effect of droplet-droplet interaction, and the variation of flame structure during the combustion of the linear arrays, are also included.

Mathematical Methods

Physical Description

Consider a linear fuel-droplet array suddenly introduced into a hot environment. Upon contact with the hot gas, the fuel droplets in the array begin to vaporize and, owing to mass loss through the evaporation, droplet size begins to decrease. The fuel vapor mixes with oxidizer from the environment to initiate the combustion process, provided the temperature in the environment is sufficiently high. The heat generated by the combustion further increases the temperature of the environment and accelerates the combustion process.

Meanwhile, as the flow develops, drag forces on the droplet surface will retard the movement of the droplets; the drag force experienced by a particular droplet depends on the droplet spacing, droplet size, and the mass transfer at the droplet surface. However, owing to wake effects, the downstream droplets usually experience a lower drag force. The difference in drag force (and thus acceleration) between the upstream and downstream droplets results in a change of droplet spacing between the droplets in the array.

In this study, the frame of reference is fixed at the center of the leading droplet. Therefore, the velocity of the leading droplet remains zero at all times and the deceleration of the leading droplet is
accounted for by adjusting the velocity of the entire flow field. The velocities of the second and subsequent droplets, with respect to the surrounding flow are corrected by their relative velocity with respect to the leading droplet.

**Assumptions**

In this analysis, the following simplifying assumptions are made to reduce computational complexity:

1. The droplet temperature is at its boiling point.
2. All the heat transferred from the gas to the droplets results in vaporization, i.e. the initial transient droplet heating is neglected.
3. Radiation heat transfer is negligible.

**Grid System**

In order to facilitate numerical calculations, the droplet array is confined in a cylindrical cell [4]. Inside the cell an embedded grid is used for the finite-difference calculations, see Fig. 1. The embedded grid consists of several spherical grids surrounding every droplet and a curvilinear grid covering the rest of flow region. The spherical grid can be regridded to follow the shrinkage of droplets at every time step [6], while the rectangular mesh between the inter-droplet spacings can be very easily redistributed to handle the change in the droplet spacings. Details of the grid and its generation have been presented earlier [9].

**Governing Equations**

The dimensional governing equations in this study are given in the following forms:

The continuity equation

$$\frac{\partial}{\partial t} (yp) + \frac{\partial}{\partial x} (ypu) + \frac{\partial}{\partial y} (ypv) = 0$$

(1)

**Momentum Equations**

**x direction**

$$\frac{\partial}{\partial t} (ypu) + \frac{\partial}{\partial x} (ypuu) + \frac{\partial}{\partial y} (ypuv) = -y \frac{\partial p}{\partial x} + \left[ y \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial (y \tau_{xy})}{\partial y} \right]$$

(2)

**y direction**

$$\frac{\partial}{\partial t} (ypv) + \frac{\partial}{\partial x} (ypvu) + \frac{\partial}{\partial y} (ypvv) = -y \frac{\partial p}{\partial y} + \left[ y \frac{\partial \tau_{yy}}{\partial x} + \frac{\partial (y \tau_{xy})}{\partial y} \cdot \tau_{**} \right]$$

(3)
where

\[ \tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \frac{2\mu}{3} \left[ \frac{1}{y} \frac{\partial (yv)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(4)

\[ \tau_{xy} = \tau_{yx} = \mu \left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right] \]  

(5)

\[ \tau_{\phi \phi} = 2\mu \frac{v}{y} \left[ \frac{1}{y} \frac{\partial (yv)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(6)

\[ \tau_{yy} = 2\mu \frac{\partial u}{\partial y} + \frac{2\mu}{3} \left[ \frac{1}{y} \frac{\partial (yv)}{\partial y} + \frac{\partial u}{\partial x} \right] \]  

(7)

Energy Equation

\[ \frac{\partial}{\partial t}(yv\rho) + \frac{\partial}{\partial x}(yv\rho u) + \frac{\partial}{\partial y}(yv\rho h) = - \left[ \frac{\partial}{\partial x}(yq_x) + \frac{\partial}{\partial y}(yq_y) \right] \]  

(8)

where

\[ q_x = -k \frac{\partial T}{\partial x} \rho \sum_{i=1}^{N} (h_i D_{i,xx} Y_i) \] , \[ q_y = -k \frac{\partial T}{\partial y} \rho \sum_{i=1}^{N} (h_i D_{i,yy} Y_i) \]  

Species Conservation

\[ \frac{\partial}{\partial t}(ypY_i) + \frac{\partial}{\partial x}(ypuY_i) + \frac{\partial}{\partial y}(ypvY_i) = \left[ \frac{\partial}{\partial x}(ypD_i \frac{\partial Y_i}{\partial x}) + \frac{\partial}{\partial y}(ypD_i \frac{\partial Y_i}{\partial y}) \right] + \alpha_i \gamma \]  

(9)

Equation of state

\[ p = pR \sum_{i=1}^{N} (Y_i / W_i) \]  

(10)
The following notation has been employed: $\rho$-density, $u$ and $v$-velocity components, $P$-pressure, $T$-temperature, $T_r$-reference temperature, $\tau$-the Newtonian stress tensor, $\mu$-viscosity, $k$-thermal conductivity, $D_i$-binary diffusion coefficient, $C_p$-specific heat, $e$-internal energy, $h$-enthalpy, $w_i$-consumption rate of the oxidized species in the reaction, $Y_i$-mass fraction of species $i$, $c_i$-stoichiometric coefficient of species $i$, $W_i$-molecular weight of species $i$, $N$-total number of species, and $R$-the universal gas constant.

It is assumed that the chemical reaction can be expressed by a one-step, irreversible reaction of the form

$$u_p F + u_0 O \rightarrow u_p P \quad (+Q) \quad (11)$$

where $F$, $O$, and $P$ are fuel, oxidizer and product, respectively.

For the source terms, it is assumed that an Arrhenius reaction occurs between fuel and oxidizer, i.e. that the reaction rate can be expressed as

$$w_i = -A[Fuel]^a[Oxidizer]^b \exp\left(-\frac{E_a}{RT}\right) \quad (12)$$

The reaction rate parameters $A$, $E_a$, $a$, $b$ for the fuels used in the present study are the same as have used by Westbrook and Dryer [10], and Dryer and Sanders [2].

**Boundary conditions**

a. at the inlet

| $u=U_m$ | $u=U_m$ , $\partial u/\partial y=0$ |
| $v=0$ | $v=0$ |
| $T=T_m$ | $T=T_m$ |
| $Y_p=0$ | $Y_p=0$ |
| $Y_o = Y_{oo}$ | $Y_o = Y_{oo}$ |
| $Y_r=1-Y_{oo}$ | $Y_r=1-Y_{oo}$ |
| $Y_p=0$ | $Y_p=0$ |

d. along the axis of symmetry

| $\partial u/\partial y=0$ | $\partial u/\partial y=0$ |
| $v=0$ | $v=0$ |
| $\partial T/\partial y=0$ | $\partial T/\partial x=0$ |
| $\partial Y_o/\partial y=0$ | $\partial Y_o/\partial x=0$ |
| $\partial Y_r/\partial y=0$ | $\partial Y_r/\partial x=0$ |
| $\partial Y_p/\partial y=0$ | $\partial Y_p/\partial x=0$ |

b. on the cylindrical envelope

| $u=U_m$ | $u=U_m$ , $\partial u/\partial y=0$ |
| $v=0$ | $v=0$ |
| $T=T_m$ | $T=T_m$ |
| $Y_p=0$ | $Y_p=0$ |
| $Y_o = Y_{oo}$ | $Y_o = Y_{oo}$ |
| $Y_r=1-Y_{oo}$ | $Y_r=1-Y_{oo}$ |
| $Y_p=0$ | $Y_p=0$ |

e. at the outlet

| $u$ is adjusted to satisfy the global mass conservation relation. | $u$ is adjusted to satisfy the global mass conservation relation. |
| $v=0$ | $v=0$ |
| $\partial T/\partial y=0$ | $\partial T/\partial x=0$ |
| $\partial Y_o/\partial y=0$ | $\partial Y_o/\partial x=0$ |
| $\partial Y_r/\partial y=0$ | $\partial Y_r/\partial x=0$ |
| $\partial Y_p/\partial y=0$ | $\partial Y_p/\partial x=0$ |
where the subscript $s$ and $\infty$ indicate surface and the ambient flow conditions, respectively.

The boundary conditions for the velocity, temperature, and species concentrations at the inlet and the outer envelop are specified for the approach flow. Symmetry conditions are applied at the axis of the array. At the outlet, the velocity component $v$ is set to be zero, the velocity component $u$ is adjusted to satisfy the global mass conservation relation (see appendix), and the rest of the flow properties are assumed to have zero gradients. The boundary conditions at the droplet surfaces are the energy-mass balance, and the mass balance for each species. It should also be mentioned that, since the downstream droplets do not have the same velocity as the leading droplet which is the reference frame, the velocity components on the surfaces of the second and third droplets are first evaluated by applying boundary conditions (c) as if the droplets are at rest with respect to the leading droplet, and the calculated velocity components are then corrected by the relative velocity of the droplet with respective to the frame of reference.

**Transport Properties**

Coefficients for viscosity and binary diffusion have been evaluated using the kinetic theory of Chapman and Enskog [11]. The thermal conductivity of each constituent was calculated from the modified Eucken model [11]. The thermal conductivity and viscosity of the mixture were calculated by the formulas recommended by Mathur, et. al. [12]. The heat capacity and the heat of formation was derived using JANAF polynomials [13].

**Numerical Scheme**

The momentum equations in this study, as shown in equations 2 and 3, are in pressure-velocity form. In this work, a numerical scheme SIMPLEM [14] (Semi Implicit Pressure Link Equation-Modified) is used to solve these equations. This numerical scheme can avoid a checkerboard flow field without adopting a staggered grid. Once the flow field is determined, the procedures for solving the governing energy and species equations are very similar to the procedures for solving momentum equations, and they can be found in Ref. 14. It should also be mentioned that the numerical scheme SIMPLEM was developed for generalized coordinates. Therefore, the governing conservation equations are first rewritten into generalized equations before they are solved in the numerical scheme. The outline of the procedures has been described earlier [9].

**The Calculation of Droplet Radius and Droplet Spacings**

The droplet radius is determined from fuel vaporization rate by

$$\frac{dR^2}{dt} = \frac{1}{\rho_i} \int_{0}^{\pi} \rho_i V_s y d\theta$$

where $\rho_i$ is the density of liquid phase.
The drag force on the droplet due to pressure and shear are given by

\[ F_p = \int p \cos \theta \, ds \]  \hspace{1cm} (14)

\[ F_F = \int (\tau_{r\theta} \sin \theta - \tau_{r\theta} \cos \theta) \, ds \]  \hspace{1cm} (15)

where \( s \) is the droplet surface area.

The total drag force is given by

\[ F_D = F_p + F_F \]  \hspace{1cm} (16)

and Newton's law of motion specifies the droplet acceleration from

\[ F_D = \frac{4}{3} \pi R^3 \rho_\text{f} A \]  \hspace{1cm} (17)

where \( A \) is acceleration of the droplets. The change of the droplet velocities is then

\[ \Delta U = A \Delta t \]  \hspace{1cm} (18)

Knowing the acceleration and the velocity of the droplets, the relative motion and the spacing change between the droplets in a array can be easily determined.

**Results and Discussions**

In the present study, droplets are evaporating and burning at a pressure of 10 atmosphere in a uniform flow. The temperature of the inflow gas (\( T_i \)) is at 1250 K. The computation has been performed for a single, isolated 100 \( \mu \text{m} \) (\( R_0 \)) octane droplet burning at an initial Reynolds number of 100, a case that has been previously studied by Dwyer and Sanders [2]. The results of the calculation are shown in Figs. 2-6. The time variation of pressure drag (\( C_p = F_p / (\rho U^2 A/2) \)) and the skin friction drag (\( C_F = F_F / (\rho U^2 A/2) \)) on the droplet surface are shown in Fig. 2 and that of total drag are shown in Fig. 3. It can be seen from these two figures that the agreement between the present results and the results of Dwyer and Sanders is very good.

The time variation of the overall Nusselt numbers, which is the average of the local Nusselt number (\( =2R(\partial T/\partial r) / T_i \)) over the droplet surface, in the present study and that obtained by Dwyer and Sanders are shown in Fig. 4. Although our predicted Nusselt number is slightly lower than that in Dwyer and Sanders' study (the reason is not yet determined), the general trends agree very well. The contours at a dimensionless time (\( =Ut/R_0 \)) of 283 are shown in Fig. 5. These contours correspond to the dimensionless time (\( =\alpha t/R_0^2 \)) of 7.86 in the study of Dwyer and Sanders [2] and, although not shown, the agreement between these temperature contours and those obtained by Dwyer and Sanders is also good. The change in droplet size and velocity is shown in Fig. 6. In this case, the droplet size decrease is almost linear with time until the droplet is about 40% of its original size. The burning rate is then slightly increased because, owing to the reduction
in intensity of the convective flow, the flame diffuses forward to enclose the entire droplet.

For a linear droplet array, we limited our computation to an arrays with a maximum of three droplets in order to reduce computational cost. The initial droplet conditions were taken to be identical to the single droplet case previously discussed, and the starting Reynolds number was also set at 100. The spacings between droplets were initially set at 14 radii. Because of the velocity difference, the spacing between the first and second droplets is steadily reduced as the computation proceeds. This will eventually lead to droplet coalescence and render the problem too complex for the present grid system. Therefore, the calculations of this study are carried out only up to the dimensionless time of 265, where the droplet spacing between the first two droplets was reduced to half of the original distance.

Figs. 7-9 show the temperature contours at dimensionless times of 7, 13, and 19, respectively. In Fig. 7, it can be seen that ignition occurs simultaneously in the region behind each individual droplet; the temperature-contour patterns behind these droplets are almost identical. Fig. 8 shows the rapid expansion of the flame zone in the inter-droplet region and the drastic change in the temperature distribution around the downstream droplets. Fig. 9 shows further expansion of the high temperature zone in the inter-droplet region. At this time the downstream droplet is almost enclosed by the high temperature gas.

Figure 10 shows the time variation of pressure drag and skin friction drag around the three droplets. In this figure, a sudden increase in pressure drag is observed during the ignition, after which the pressure drag tends to stabilize. A similar variation in the pressure drag during ignition has also been reported by Dwyer and Sanders [3]. The sudden increase in the pressure drag, as discussed by Dwyer and Sanders, is triggered by the rapid change in the temperature and density around the droplets. Notice that the pressure drag for the second and the third droplets is almost identical, and is lower than that of the first droplet. The drag reduction for the downstream droplet owes to the decrease in the droplet surface pressure. For the skin friction drag, the variation is quite smooth, compared to the pressure drag variation. Because of the higher temperature gradient and faster evaporation, the shear stress or the skin friction for the second and third droplets is more significantly reduced than that of the first droplet.

Figure 11 shows the Nusselt number variation with time for the three droplets. For the first droplet, despite the ignition, the Nusselt number decreases with time. This owes to the strong convective flow that prevents the flame zone from diffusing to the droplet; therefore, the leading droplet behaves like an evaporating droplet and has a lower burning rate than the other droplets. For the downstream droplets, owing to the development of the flame zone in the inter-droplet region during the ignition process (see Figs. 9-11), the Nusselt numbers around the second and third droplet are drastically increased. It is also noted that during the entire calculation, the overall Nusselt number is slightly decreased for all three droplets after the ignition period. This is attributed to the reduction of the Reynolds number.

Figures 12 and 13 show the time variation of droplet size and velocity for the three droplets in the array. Figure 12 shows that, during the time interval of this calculation, only about 10% of the fuel mass in the leading droplet was consumed, and about 14% in the second and third droplets was consumed. It also shows that the variation of the droplet size with time is almost linear for these three droplets, and that the
variation of the droplet size for the second and the third droplet is almost identical. Fig. 13 indicates that, owing to the drag force on the droplet surface, the velocity of leading droplet is reduced to 82 percent of the initial value, and that the velocities of the second and the third droplets are reduced to about 87 percent of their initial values. Here again, the time variations of velocity for the downstream droplets are almost identical. We conclude that, for the time span considered here, an asymptotic behavior does emerge for the downstream droplets. Fig. 14 show the spacing variation for the array. In this figure, the spacing between the leading droplet and second droplet is reduced to 6 radii at time of 265, while the spacing between the second and the third droplet varies only slightly.

Figure 15a shows the temperature contours for an the array burning at a dimensionless time of 55. At this time, the dimensionless droplet velocity for the first, second, and third droplet is 0.956, 0.966, and 0.967, and the dimensionless droplet sizes are 0.972, 0.966, 0.967, respectively. The droplet spacing between the first two droplets is about 13.8 radii and that between the second and the third droplets is 14. The continuous flame layer around the downstream droplet indicates the flame is fully developed. This flame layer also accounts for the high Nusselt number for the downstream droplets as seen in Fig. 11. Notice that the temperature distribution patterns around the second and the third droplet are very similar. This explains the great resemblance in the overall Nusselt number for these two downstream droplets seen in Fig. 11. Figure 15b shows the fuel mass fraction contours corresponding to the same droplet array. From this figure, the fuel mass fraction around the second and the third droplets is seen to be higher than that around the first droplet. This is partly because the remaining fuel vapor from the upstream droplet is swept to the vicinity of the downstream droplet, and partly because the hot gas around the two downstream droplets causes a significant amount of fuel to evaporate from the droplet surface.

Figure 16a shows the array burning at t=165. At this time the droplet velocity for the first, second, and third droplet is 0.884, 0.918, and 0.920 and the sizes are 0.930, 0.911, 0.913, respectively. The droplet spacing between the first two droplets is about 11.5 radii and that between the second and the third droplets is 13.8 radii. It is interesting to note that the droplet spacing between the first and the second droplets is significantly reduced, while the spacing change between the second and the third droplets is negligible. Also, the flame zone between the first and the second droplet is shrinking because of the forward displacement of the second droplet, while the flame zone between the second and the third droplets does not change much from what is seen in Fig. 15a. The fuel mass fraction contours corresponding to the same array is shown in Fig. 16b.

Figure 17a shows the array at a dimensionless time of 265. At this time, the droplet velocity for the first, second, and third droplet is 0.811, 0.869, and 0.873 and the droplet sizes are 0.885, 0.852, 0.854, respectively. The droplet spacing between the first two droplets is about 6.3 radii and that between the second and the third droplets is 13.5 radii. Compared to Fig. 16a, the droplet spacing between the leading and the second droplet seen in this figure is reduced further, and the flame zone is almost forced out of the region. It is also interesting to note that, despite the significant change in spacing between the first and the second droplets, the burning behavior of the second droplet does not deviate much from that of the third droplet (see Fig. 11). This is in contrast to the conclusions drawn from a heat transfer study for a solid sphere array [4,5] and the evaporation study for a liquid droplet array[ 6,7]. In those studies, the relative cold flow
(or vapor) from the upstream droplet is carried to the vicinity of downstream droplets and leads to a temperature drop around those droplets, thus causing a reduction in the heat transfer or evaporation rate; the reduction is increased as the spacing is decreased. However, in this study, a thick flame layer in the inter-droplet region between the first two droplets is developed by the heat released from the combustion of fuel vapor. Since the temperature distribution inside the flame zone is quite uniform (see Fig. 15a), the environment experienced by the second droplet during its forward displacement is not significantly altered. Therefore, the burning rate of this droplet remain unchanged. Of course, if the droplet spacing is further reduced, the mass amount of cold fuel vapor accumulated at the inter-droplet spacing would extinguish the flame. Thus the burning rate of the second droplet would be significantly reduced. This has been shown in the results of our previous study [8]. Finally, the fuel mass fraction contours corresponding to this array are shown in Fig. 17b.

Conclusions

In the present study, the burning of a linear, three-droplet array in a parallel convective flow has been studied numerically. The detailed, time-varying droplet burning behavior has been described. The decrease of droplet size due to evaporation, and the velocity change due to drag force are considered in this study. The calculations are first carried out for a single, isolated droplet, and the results are compared to those of Dwyer and Sanders for the same case. The agreement between these two studies is good.

For the multiple-droplet array, because of incipient coalescence between the first droplet and the second droplet, the calculations are carried out only until about 10 percent of the initial mass of the first droplet is consumed. In this study, it is found that, at the beginning of droplet burning, ignition occurs simultaneously behind each individual droplet. For the time interval studied, the droplet-droplet interaction does not reduce the burning rate of the interacting droplets as originally presumed. Rather, the downstream droplets have a higher burning rate because they are located inside a thick layer of flame from the preceding droplets. Owing to the constant change in the droplet spacing, the flame structure around the array varies during the burning process.

Over the time interval considered here, however, no significant alteration in the burning behavior of the second droplet, in comparison with the third droplet, was detected. This is so even though the spacing between the first and second droplet was reduced by half. This apparent asymptotic behavior of the downstream droplets justifies the small number of droplets used in this study. Furthermore, the asymptotic behavior provides a quantitative limit for droplet combustion rates with maximum droplet interaction; the single droplet results provide the other limit for minimum interaction effects. The combustion rates for droplets in a complex three dimensional spray should fall somewhere between these two limits.

In order to study more complete droplet burning behavior in an infinite linear array or in a spray, it may be worthwhile to study a droplet arrays of four droplets with a fixed droplet spacing. The inclusion of the fourth droplet will further ensure asymptotic behavior in temperature and species distribution around the downstream droplets, and the assumption of constant droplet spacings will exclude the possibility of
coalesce between droplets, thus enabling the calculation to be performed for a much longer time interval than in the present case. By assuming an uniform velocity for all the droplets (the uniform velocity being the average velocity of the second, third, and fourth droplets), a droplet burning at low Reynolds numbers can then be studied, and the burning behavior observed for the downstream droplet should give an even better approximation for the typical droplet burning behavior in a spray.

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References


Figure 1. Embedded grid for the present study.
Figure 2. Computed pressure drag and skin friction drag coefficients in comparison with the pressure drag coefficient calculated by Dwyer and Sanders.

Figure 3. Comparison of the computed total drag coefficient with that calculated by Dwyer and Sanders as well as that by a quasi-steady correlation.
Figure 4. Comparison of the computed Nusselt number with that calculated by Dwyer and Sanders.

Figure 5. Isotherms in the gas phase at dimensionless time of 283. At this time the gas phase Reynolds number is 69.5 and the droplet radius is 0.88 \( R_0 \).
Figure 6. Time variation of droplet size and velocity for the single, isolated droplet.
Figure 7. Isotherms in the gas phase at dimensionless time of 7.

Figure 8. Isotherms in the gas phase at dimensionless time of 13.

Figure 9. Isotherms in the gas phase at dimensionless time of 19.
Figure 10. Time variation of drag coefficients for droplets in the array.

Figure 11. Time variation of Nusselt number for droplets in the array.
Figure 12. Time variation of droplet sizes for droplets in the array.

Figure 13. Time variation of droplet velocities for droplets in the array.
Figure 14. Time variation of droplet spacings for the array.
Figure 15a. Isotherms in the gas phase at dimensionless time of 55.

Figure 15b. Fuel mass fraction contours in the gas phase at dimensionless time of 55.
Figure 16a. Isotherms in the gas phase at dimensionless time of 155.

Figure 16b. Fuel mass fraction contours in the gas phase at dimensionless time of 155.
Figure 17a. Isotherms in the gas phase at dimensionless time of 265.

Figure 17b. Fuel mass fraction contours in the gas phase at dimensionless time of 265.
Chapter 9

Summary and Conclusions

In previous chapters, a number of models have been proposed -- the potential flow model (Chapter 4), the Stokes flow model (Chapter 5), and the viscous flow model (Chapter 6, 7, and 8). Although all these models have been developed to simulate the combustion and/or transport phenomena for linear droplet arrays in a co-axial, convective flow, they use different assumptions and have been applied for different flow conditions. Consequently, the results of these models differ. Since, in this thesis, each model is presented as an independent chapter, the differences between these models are not clearly shown. In this chapter, the results of these models will be briefly summarized and compared in order to provide a more global view.

Potential Flow Model

In the potential flow model, the fluid density is assumed to be constant and a thin flame sheet is assumed. This model shows that, at the droplet spacing used, the leading droplet is not affected and the burning rate of the downstream droplets is reduced owing to the droplet-droplet interaction. The droplet interaction is shown to be greater for a droplet array with smaller droplet spacing. The model has also been applied to arrays with a large number of droplet, and an asymptotic behavior is observed as the number of droplets increases. The advantage of this model is that the computational procedure and the computer time required for each iteration is small compared to the rest of the models. However, the accuracy of this model is not yet known, and the results should be compared with the experimental data in the future in order to determine the adequacy of this model as an approximation for "real" systems.

Stokes Flow Model

In the Stokes flow model, constant fluid properties and infinitely-fast reaction kinetics (flame sheet) are assumed. Since this model is developed for a low Reynolds number region, the heat and mass transfer in the fluid is controlled by conduction and diffusion. Consequently, the isotherms and the contours of each specie spread far away from the linear arrays and a large computational domain is, therefore, usually necessary for this model. The model was first applied to a mass transfer calculation that appeared previously in the literature, and the agreement between our calculations and the published results is very good. The model was then applied to the combustion of a linear droplet array. The results show that, at a very low Reynolds number region, the interaction between droplets is small for arrays with large droplet spacing, and thus the burning rate around the droplet surface is almost uniform. However, at a small droplet spacing, because of the lack of a dominate convective flow, the vapor emitted from the downstream droplet can interact with vapor around the rear hemisphere of the upstream droplet and, therefore, reduce the burning rate around the rear hemisphere of the upstream droplet. Since this model uses an existing analytical solution for the flow field, the computational procedure is simplified and the computational time required is greatly reduced, compared to the other viscous flow model proposed in this work. However, it is suitable only for droplet arrays in a very low Reynolds number flow regime.
Viscous Flow Heat Transfer Model

A complete model to describe the droplet burning at an intermediate Reynolds number region involves great complexity, and so far no experimental data are available for model validation. However, experimental data on the heat transfer of a solid sphere in a convective flow are available in the literature. Therefore, it was deemed desirable to develop a heat transfer model for solid spheres as an intermediate step, and to use existing experimental data to validate the heat transfer model. A numerical scheme SIMPLEM is used to solve the momentum equations, and the results of this model for a single sphere agree very well with published experimental data. Calculations were also performed for an array with three droplets. Although this model can provide an accurate results for the heat transfer from solid spheres, it requires a significant amount of computer time and its calculation procedures are far more complicated than the models previously discussed.

Steady-State Combustion Model

The model we proposed for the steady-state combustion calculation of a linear droplet array is an extension of the model for viscous flow heat transfer calculation. In this model variable transport properties and a finite-rate chemical reaction have been included. The calculations were first performed for a single, isolated octane droplet, and the results of our calculation agree very well with the published results of other investigators. This model was then applied methanol arrays. The results indicate that the model of single droplet is not adequate to describe the typical droplet burning behavior in a spray. For instance, the single droplet model predicts the burning rate in a highly convective environment is lower than that of a droplet burning in a highly diffusive environment because the flame zone is blown behind the droplet by the strong convective flow. Our results shown that this is also only true for the leading droplet in a linear array. For the downstream droplets in an array, however, the strong convective flow pushes the flame zone closer to the droplet surface and, consequently, increases their evaporation rate. When our model is applied to droplet arrays with large droplet spacing and a Reynolds number of about 10, an asymptotic behavior in the droplet burning pattern emerged. Similar asymptotic behavior has also been observed for arrays with a large number of droplets in our previous potential flow model and Stokes flow model. This asymptotic behavior, in our opinion, will be a better approximation of the burning behavior of a typical droplet in a spray than can be obtained from a single-droplet model.

Although this model can provide detailed information on the droplet burning behavior in a linear array, the computer time it requires is extensive. It takes approximately 20 to 30 hours of CPU time in a Floating Point System (FPS) 264 for a typical run. The reason for this strong demand in computer time is that: 1) a set of mass balance equations is needed to describe the mass fraction of each specie in the physical domain and, because numerous species are involved in the combustion process, the computation is greatly increased; 2) since variable transport properties are used at every node, many computations are needed to update these properties at each iteration; and 3) the number of iterations needed to reach a converged solution is increased owing to large temperature variations occurring in a short physical distance between the droplet surface and the flame zone.
Unsteady-State Combustion Model

The steady-state model describes a burning droplet array with fixed droplet spacing at fixed Reynolds number. Although this model provides information on the effects of droplet spacing and the convective flow on the burning rate of the droplet array, it does not fully describe the real droplet burning process. For instance, in reality, the sizes of droplets in an array are shrinking as time progresses. After a period of time, as the droplet size is reduced and droplet spacings become relatively large, the flame structure in the inter-droplet spacing can change. At the same time, the droplet velocity is reduced owing to the drag force acting on the droplet surface, and the burning environment can change from being highly convective to a diffusion controlled. For such a complicated system, the droplet burning behavior can be accurately described only through an unsteady-state model. The transient model in this work can be regarded as an extension of the steady-state model. However, in this model the unsteady time term is included as well as the variation of droplet spacing due to the drag force differences and the droplet size change resulting from evaporation. Once again, the calculation of this model is quite intensive. It requires about 50 hours of CPU time in a Floating Point System (FPS) 264 for an typical run. The computational results show that at the Reynolds number (Re=100) and initial droplet spacings (14 radii) used, coalescence between the first two droplets occurs in the early stage of droplet burning, when only 10% of fuel mass has been consumed. The results also indicate that, despite a significant change in the droplet spacing between the first two droplets, the burning behavior of these two droplets does not change much. This is because the temperature of thick flame layer is quite uniform in the inter-droplet spacing; therefore, the environment around the downstream droplets does not change very much when they are moving forward during the
In this chapter, a few future research directions are proposed for the continuation of the present work. They are listed and briefly discussed below.

**The Extension of the Potential Flow Model and Stokes Flow Model**

The potential flow model and Stokes flow model require less effort in development and less computer time for computations. Owing to their simplicity and computational economy, these models could be useful for practical application, providing they furnish reasonable approximations to real system behavior. Good qualitative agreement with experimental data has been obtained by Sangiovanni and Labowsky[1] using method of images (M.O.I), a method also based on potential flow theory, to simulate the burning time of linear fuel droplet arrays in quiescent atmosphere. Thus we expect that the present potential flow model and Stokes flow model can be extended to an unsteady-state model to calculate the droplet lifetime history. The results of droplet size variation with time can then be compared with existing experimental data (for the Stokes flow model) or data that is yet to be collected (for the potential flow model).

**Transient Heat and Momentum Transfer Inside Droplet Liquid**

The burning rate of droplets is essentially determined by the evaporation from the liquid droplet surface. The evaporation is dominated by the temperature gradient around the droplet surface as well as the heat and momentum transfer inside the liquid droplet. Therefore, in order to predict the burning rate of a droplet more accurately, it is necessary to understand the transient heat and momentum transfer inside a liquid droplet. The heat and momentum transfer processes inside the droplet include: 1) internal circulation induced by shear stress at the gas-liquid interface, and 2) heat transfer inside the droplet. Some earlier studies of these two key factors have been carried out analytically and numerically by Prakash and Sirignano [2,3]. They assumed the convection process dominated the heat transfer within the droplet. However, the recent studies by Dwyer and Sander [4,5] indicate that, during the lifetime of a fuel droplet, the process transforms from convection dominated to conduction and diffusion dominated. Therefore, they concluded that in order to accurately describe the process, a complete set of energy equations which include all the convective and conductive terms, should be employed. The most recent research conducted in this subject is by Patnaik [6]. He studied the droplet lifetime history of evaporating fuel droplets with transient droplet heating for one and two droplet cases by solving a complete set momentum and energy equations for the gaseous phase around the droplets and the condensed phase inside the fuel droplets. So far, however, no study has yet been undertaken to include droplet heating in the droplet lifetime history for the combustion situations.

Since the droplet burning process includes ignition, burning, and extinction, the entire droplet lifetime history can be quite different from that of an evaporating droplet, and the results for the evaporating
droplet cannot be used, in general, for burning droplet case. Therefore, some additional work for a burning droplet with transient heating in the liquid phase needs to be carried out. The work to simulate such a system can be very easily achieved by solving the momentum and energy equations in the liquid phase in a way very similar to that used for the gas phase. In addition, a momentum balance between the liquid phase and gas phase needs to be set up to calculate the tangential velocity component on the droplet surface. The details for setting up the required equations can be found in Patnaik’s work [6]. This model should enable us to evaluate more realistically the droplet burning time.

The Combustion of Multicomponent Droplets

Another common practice to enhance or reduce the burning rate of droplets is to add another component to the liquid first. The added component can have drastic effect on ignition, extinction and incineration of the liquid droplet, and it sometimes even causes microexplosions [7]. For instance, the study of Aggarwal [8] indicates the ignitability of a fuel spray can be greatly increased by the presence of a second, more volatile component. On the other hand, the study of Sorbo, et al. [9] on the incineration of chlorinated alkane droplets indicates that a less volatile additive could drive out a substantial part of the more volatile liquid in the early droplet life and, as the droplet size diminishes, the combustible additive would become more concentrated to sustain the burning. They concluded that relatively less volatile additives can enhance the droplet burning rate and promote more complete burning out of the droplet.

Despite the importance of additives to the incineration of liquid droplets, very few theoretical studies on this topic have appeared in the literature. The work by Tong and Sirignano [10,11] are the most recent studies on multicomponent droplet vaporization. Their studies are, however, over simplified. For example, the governing equation is simplified to a one-dimensional similarity solution and transport physical properties are assumed to be constant. Furthermore, their model was applied only for the evaporation of a single, isolated droplet; no combustion was included. Therefore, some additional investigation in this subject should be carried out in the future. The extension of our current models will involve additional species to be accounted for in the gas phase. The solution procedure for these equations will remain the same as that employed for the single component case studied here. But species equations must be solved in the liquid phase as well. One species equation is needed in the liquid for each new component. Boundary conditions at the sphere surface can be obtained through Raoult’s law. It is our belief that the results of this study will not only significantly increase the knowledge on the mechanism of the combustion of multicomponent liquid droplets, but will also provide the information for the choice of appropriate additive for better destruction of liquid droplets.
References


Appendix A

Experimental Methods

In view of the scarcity of experimental data in the literature on the combustion of interacting droplets in a convective flow, some experimental work in parallel with our theoretical study was also carried out, with the intention to provide data on the droplet burning rate and to study the key parameters that dominate droplet combustion, such as the effect of droplet temperature, ambient oxygen concentration, droplet size and spacing, and relative droplet and gas velocities. Despite a considerable expenditure of effort, no significant progress was made. In this chapter, a brief description of our experimental facility and methods will be given, along with an identification of the principal difficulties that limited experimental progress and some recommendation on how these problems may be solved.

Experimental Set-Up and Procedure

A. Overview

The basic experimental facility consists of 1) a rectangular flat-flame burner, 2) droplet generators, and 3) optical imaging equipment.

The general procedure is to inject droplets across the post combustion region of the burner, and to measure ignition delay time, the size and velocity history of the droplets, and droplet lifetime. Variables include flame temperature and ambient oxygen concentration as well as the composition, size, velocity, spacing, and initial temperature of the droplets.

B. Apparatus

1. Flat-Flame Burner (see Fig. 1)

The design of the rectangular flat-flame burner was based on our observations of the burners used at the Combustion Research Facility, Sandia National Laboratories, Livermore. The flame is supported on a water-cooled, sintered brass plate which, in turn, covers a 2 x 11-in honeycomb with 1/32-in cells. The burner is currently fired with methane-oxygen-nitrogen mixtures.

In previous work on the burning of linear fuel droplet arrays, the droplets were injected through the face of a conventional flat-flame burner in the direction of the gas flow (for example, Sangiovanni and Labowsky, 1982). As mentioned above, droplet interactions, as evidenced by increased burning times, were found to be important for droplet spacing as great as 25 droplet diameters.

The conditions in our system differ from the above study in one essential way: since the droplet trajectory is normal to the gas flow, vapor and combustion products in the droplet wake are largely swept from the path of a following droplet.
The selection of a droplet trajectory normal to the gas flow provide two advantages over previous experiments:

1) The effect of droplet-droplet interactions will be minimized when the slip velocity is high. In contrast, the parallel injection used in previous experiments will maximize these interactions. Thus a lower bound on the effect of interactions, under conditions more characteristic of highly turbulent flows, can be established to compliment previous results.

2) The wake effect (or its absence) can be altered by varying the slip velocity. Thus measurements between the two limits of droplet interaction are possible.

Provision has also been made for preheating the injected liquid in order to observe droplet ignition characteristics near the ignitable limit. Saitoh, Ishiguro, and Niioka (1982), as mentioned above, have found that when the droplet temperature is high, ignition occurs more rapidly as the droplet diameter increases, a result in contrast with usual concepts.

2. Droplet Generators (see Fig. 2)

Droplets are formed from vibrating jets in order to control droplet spacing. We have adopted drawn capillary tubes as nozzles, since a wide range of jet diameters is possible with these simple, inexpensive nozzles. The capillary tube is fixed to one end of a flat, rectangular piezoelectric bimorph, which is cantilevered by firmly clamping the other end. The application of a periodic voltage across the faces of the bimorph sets it into vibration in a plane normal to the nozzle axis and drives the jet to breakup at the vibration frequency. By varying the frequency, at a given jet velocity, the spacing and size of the drops can be varied over a limited range. The choice of jet diameter, jet velocity, and vibration frequency provides a broad and continuous range of droplet size, velocity, and fundamental spacing.

If only polar liquids were to be used, a single nozzle would be sufficient to obtain variable drop spacing. Droplet could be charged and then deflected into a collector by passing them through the electrostatic field produced between two plates, across which a voltage is applied. By eliminating the charge on a single droplet, its trajectory would be unaffected by the electrostatic field, and it would bypass the collector. Thus every 2nd, 3rd, 4th, or nth droplet could be directed into the test section.

To investigate non-polar liquids, two nozzles must be used, one for the non-polar test liquid and one for a polar control liquid. The non-polar droplets are directed horizontally into the test section and the polar droplets directed vertically downward. The trajectory of polar droplets is controlled by the electrostatic deflection plates so as to collide with and alter the trajectory of the non-polar droplets. If the charge on every nth polar droplet is removed, every nth non-polar droplet will pass into the test section. This procedure has been used by Sangiovanni and Labowski (1982) and Muholland et al. (1988).
3. Optical Imaging Equipment

Optical imaging is used for two purposes: 1) to monitor the operation of the droplet generators, and 2) to record images of droplets in the combustion zone.

The dual droplet generators require very fine control for proper operation. We monitor continuously the collision region of the two droplet streams by video imaging. An acoustico-optical modulate is used to drive a low-power HeNe laser beam at the same frequency that is used to drive the droplet generators. Since this frequency (10-20 kHz) is much greater than the scan rate of the video, the modulated laser beam strobos the droplets and multiple, “frozen” droplet images are superimposed on the vidicon tube. This system also provides a means to measure initial droplet size and velocity.

To record images of the droplets in the combustion zone, we use single flash still photography. Droplet diameters are measured directly from enlarged projections of the film image. This technique has been used successfully by Sangiovanni and Labowski (1982) and Law (1984), although in these studies the droplet sizes were larger. The residence time at any particular location is calculated from the distance and droplet velocity (see Fig. 3).

Initial Observations and Recommendation

A. Initial Observations

Our initial observations have been made with 250 μm octane and ethyl alcohol droplets initially at room temperature. For the conditions used, individual droplet ignition does not occur. Rather, a continuous flame front is located above of and approximately parallel to the droplet trajectory.

This behavior is in sharp contrast to the observations of Sangiovanni and Labowski, who observed individual droplet ignition when the droplets were injected in the same direction (and at the same velocity) as the combustion gas flow. The difference illustrates the strong convective effects on droplet burning behavior.

B. Technical difficulties and Recommendations

Two major difficulties encountered in this experimental work are:

1. Inaccuracy of the charging device.

One of the problems we have encountered with our droplet generator is that the charging ring does not charge precisely only the selected droplet as designed. Instead, it charges the neighboring droplet as
well. Although an attempt has been made to vary the size, the shape, or even the material of the charging ring, the situation has not improved. Therefore, we suspect that the problem lies in the electronic control device that was designed, built, and used to send the charging pulse to the charging ring. We believe that, because the duration of the pulse is too long, it charges two droplets at same time. Therefore, we recommend that the control device be redesigned so that the pulse used to charge the droplet is of adjustable duration.

2. Insufficient residence time for droplet in the combustion zone

During the operation, the initial droplet velocity is about 2-3 m/s. Although a thick layer of flame can be observed, no significant reduction in droplet size can be detected. When the liquid droplets heat up, their volume expands and this expansion offsets the volume reduction through the evaporation. Therefore, in order to obtain a greater volume reduction, the droplet must burn more quickly, or the residence time for the droplets must be increased.

To make the droplet easier to burn, we first reduced the droplet size, but we soon found that, if the droplet size is less than 100 μm, it is almost impossible for our photo-equipment to get a clear image of the droplets. Another approach we adopted was to preheat the fuel liquid. The problem with this approach is that, once the liquid is heated, its density and surface tension change. This causes tremendous problems in forming two identical droplet streams, rendering our droplet generation technique unusable. We also attempted to raise the ambient temperature by increasing the oxygen flow rate in the flat-flame burner. Although vigorous burning on the flat-flame burner was achieved by increasing the oxygen, this burning also caused some vibration on the droplet array. This slight vibration of the arrays made the focusing extremely difficult. Therefore, to this point, we conclude that an increase in the residence time of the droplet is more feasible than increasing the burning rate.

One way to increase the residence time is to reduce the droplet velocity. However, for the experimental set-up used in our laboratory, the reduction in the droplet velocity will cause an increase in the gravity-induced droop of the trajectory. A curved droplet trajectory, however, makes imaging and data interpretation more difficult.

Since the major problems of this experimental work are related to the trajectory of the droplet array, we recommend that the droplet generator be re-oriented to allow the droplet array to move vertically. This will not only eliminate the trajectory variation during the combustion process, it will also allow a wide range of droplet velocities.
References


Figure 1. Orientation of droplet trajectories with respect to the rectangular burner.
Figure 2. Schematic representation of the droplet generator system.
Figure 3. Video and photographic imaging scheme for measurement of droplet size and residence time.

\[ v = \lambda_0 f \]

\[ v(t) = \lambda(t) \cdot f \]

\[ t = N/f = L/v \]

\[ \dot{m} = \rho \Delta V / \Delta t \]

\[ \eta(\lambda) = \dot{m}(\lambda) / \dot{M} \]
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