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VAPORIZATION OF SYNTHETIC FUELS

Final Report

By
W. A. Sirignano
S. C. Yao
A. Y. Tong
D. Talley

November 1983

Work Performed Under Contract No. FG22-81PC40277

Carnegie-Mellon University
Department of Mechanical Engineering
Pittsburgh, Pennsylvania

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**FINAL REPORT
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Foreword:

For some time now, the Department of Mechanical Engineering at Carnegie-Mellon University has been studying the vaporization of synthetic fuel droplets via a joint theoretical-experimental program sponsored by DOE Pittsburgh Energy Technology Center with Mr. James Hickerson as the DOE monitor. This program originally was intended to be a three-year effort but only about one-half of the funds were committed before the DOE Synthetic Fuels Program was curtailed. For that reason, the experimental program was not completed and only limited experimental data and limited comparison between theory and experiment has resulted.

A list of publications generated under this program follows:

A.Y. Tong, "Advancements in the Theory of Transient Vaporization of Fuel Droplets with Slip and Internal Circulation," Ph.D. Thesis, Carnegie-Mellon University, Dept. of Mechanical Engineering, August 1983.

W.A. Sirignano, "Fuel Droplet Vaporization and Spray Combustion Theory," to appear in *Progress in Energy and Combustion Science*, 1984.

A.Y. Tong and W.A. Sirignano, "Analysis of Vaporizing Droplet with Slip, Internal Circulation, and Unsteady Liquid-Phase and Quasi-Steady Gas-Phase Heat Transfer," *Proceedings of ASME-JSME Thermal Engineering Joint Conference*, Vol. 2, pp. 481-487 (1983).

W.A. Sirignano and A.Y. Tong, "Analytical Solution for Diffusion and Circulation in a Vaporizing Droplet," *Proceedings of Nineteenth Symposium (International) on Combustion*, Combustion Institute, pp. 1007-1020 (1983).

This final report is written in two volumes. The first volume presents the theoretical effort and was drafted by Dr. A.Y. Tong while the second volume presents the experimental work and was drafted by Mr. D. Talley. Professors Sirignano and Yao reviewed both volumes and contributed to the revisions.

ABSTRACT

The problem of transient droplet vaporization in a hot convective environment is examined. The main objective of the present study is to develop an algorithm for the droplet vaporization which is simple enough to be feasibly incorporated into a complete spray combustion analysis and yet will also account for the important physics such as liquid-phase internal circulation, unsteady droplet heating and axisymmetric gas-phase convection. A simplified liquid-phase model has been obtained which is based on the assumption of the existence of a Hill's spherical vortex inside the droplet together with some approximations made in the governing diffusion equation. A one-dimensional gas-phase model which simplifies the analysis in the gas phase through representing the heat and mass transfer rates by an optimum average for the stagnation point region and the shoulder region of a droplet has been obtained. The results from coupling this simplified gas-phase model to the simplified liquid-phase solution are in good agreement with the results of a more detailed model. The present simplified model requires significantly less computing time than the more detailed model.

The use of the simplified model in a spray situation has also been examined. It has been found that droplet heating and vaporization are essentially unsteady and droplet temperature is nonuniform for a significant portion of its lifetime. The effects of different gas-phase and liquid-phase models on the vaporization behavior for a single isolated droplet as well as in a spray condition have been studied. The feasibility of incorporating the present simplified model into a one-dimensional spray vaporization calculation has been verified which demonstrates the potential usefulness of the model in an overall spray situation. It has been found that the droplet vaporization characteristic can be quite sensitive to the particular liquid-phase and gas-phase models.

The simplified model has been extended to the multi-component droplet case. The results of the present simplified model are compared with the results of infinite diffusivity model and spherical diffusion limit model. Largely due to the neglect of the thermal and mass diffusion resistances, substantial differences in the vaporization behaviors between the infinite diffusivity model and the other two models are found.

At short times, the disagreements between the models are caused by the difference in the mode of the thermal energy transfer. While for the bulk of the droplet lifetime, the discrepancies are due to the difference in the mass diffusion models. The disagreements between the present simplified vortex model and the spherical diffusion limit model are comparatively less.

Both the finite difference solution scheme and the ordinary differential equation formulation have been used for the coupled vaporization problem. The computational efficiencies of the two solution schemes are compared. The ordinary differential equation formulation which eliminates the spatial dependence from the problem has been found to be more efficient.

The results of the various models are compared with the existing experimental data. Due to large scattering in the experimental measurements, particularly the droplet diameter, no definite conclusion can be drawn based on the experimental data.

Finally, certain research problems which are related to the present study are suggested for future studies.

ACKNOWLEDGEMENTS

More than a formal thank you is deserved by my thesis advisor, Professor William A. Sirignano, for his care, guidance and help provided throughout the course of the study. His helpful suggestions and brilliant insights were crucial for the completion of this thesis.

Thanks are also extended to all the thesis committee members who were kind enough to serve on the committee. A special word of thanks goes to Professor Fletcher J. Osterle for his sincere guidance and help in the last four years.

The professional appearance of this thesis is due to Mrs. Darlene Kopriva. Her diligent typing of the difficult text is appreciated.

Finally, I would like to thank all of my friends at the department for just being fine people to be associated with. The experience will never be forgotten.

TABLE OF CONTENTS

Nomenclature	0
1. INTRODUCTION	1
1.1. Importance of Droplet Vaporization Study	1
1.2. Objective of this thesis	1
1.3. Approach Adopted in this Research	2
1.4. Organization of Thesis	3
2. Literature Reviews on Single Droplet Vaporization Theories	4
2.1. Spherically Symmetric Models	4
2.1.1. d^2 Law Model	4
2.1.2. Infinite Conductivity Model	6
2.1.3. Conduction Limit Model	7
2.2. Droplet Vaporization with Convective Effects	9
2.2.1. Ranz-Marshall Model	9
2.2.2. Prakash and Sirignano's Axisymmetric Model	10
3. Liquid-Phase Analysis	13
3.1. Removal of the Thermal Boundary Layer	13
3.1.1. Introduction	13
3.1.2. Importance of the Two-Dimensional Representation of the Thermal Boundary Layer and the Quasi-Steadiness Assumption	14
3.1.3. Results and Discussions	16
3.1.4. Summary	20
3.2. Unsteady Thermal Core Analysis	20
3.2.1. Introduction	20
3.2.2. Thermal Core Solution	21
3.3. Results and Discussion	29
3.4. Summary	32
4. Quasi-Steady Gas-Phase Analysis	34
4.1. Introduction	34
4.2. Gas Phase Analysis	34
5. Solution of the Coupled Problem	40
5.1. Introduction	40
5.2. Finite Difference Solution	41
5.3. Ordinary Differential Equation Solution via Integral Equation Formulation	46
6. Multicomponent Fuel Droplets	54
6.1. Introduction	54
6.2. Extension of the Single-Component Droplet Analysis and the Finite Difference Solution	57
6.2.1. Extension of the single-component droplet analysis	58
6.2.2. Finite difference solutions	61

6.3. Ordinary differential equation via integral equation formulation	69
7. One Dimensional Spray Vaporization Study	81
7.1. Introduction	81
7.2. Physical Situation and Mathematical Formulation	81
7.3. Solution Procedure	85
8. Comparison of Vaporization Models	87
8.1. Introduction	87
8.2. Spherically Symmetric Models	88
8.3. Droplet Vaporization With Convective Effects	89
8.4. One Dimensional Spray Vaporization	91
8.5. Summary	94
9. Comparison With Experimental Data	97
9.1. Available Experimental Data	97
9.2. Experimental Comparison Procedure	99
9.3. Results and Discussions	100
10. Conclusions, Discussions and Future Work	104
10.1. Conclusions and Discussions	104
10.2. Future Work	107
References	109
Appendix A. Coupled Gas-Liquid Solution in the Non-Vaporizing Droplet Case I - Integral Equation Solution	113
Appendix B. Source/Sink Terms in the Gas-Phase Equations of the One- Dimensional Spray Vaporization Formulation	116
Appendix C. Coupled Gas-Liquid Solution in the Non-Vaporizing Droplet Case II - Series Solution	118
Appendix D. Series Solutions for the Uncoupled Liquid-Phase Thermal Diffusion Equation With Zero C	125
Appendix E. Series Solutions for the Uncoupled Liquid-Phase Thermal Diffusion Equation With Constant C	131
Appendix F. Variable Transformation for the Uncoupled Liquid-Phase Thermal Diffusion Equation with Time Varying Coefficient C	140
Appendix G. Series Solutions for the Uncoupled Liquid-Phase Thermal Diffusion Equation With Time Varying C	146
Figures	156

LIST OF TABLES

Table 5-1:	Percentage Disagreement Between the Two Models	45
Table 8-1:	Values of Various Parameters Used in Spray Calculations	95
Table 8-2:	Properties of the First Droplet Group for Different Liquid Phase Models	96

NOMENCLATURE

A	variable related to the vaporization mass flux; defined by Equation (4.4) also is the strength of the Hill's vortex (See Equation (3.7))
B'	modified Spalding transfer number
C_p	specific heat at constant pressure
f	Blasius function
g₁	dimensionless function as defined by Equation (3.8)
g₂	dimensionless function as defined by Equation (3.9)
h	sensible enthalpy of the gas mixture
h_ξ	scale factor in the streamwise direction
h_γ	scale factor in the direction normal to the streamline
h_n	scale factor in the azimuthal direction
i	$(-1)^{1/2}$
J₀	Bessel function of the first kind and order zero
J₁	Bessel function of the first kind and order one
k_g	thermal conductivity in the gas phase
k_l	thermal conductivity in the liquid phase
L	heat of vaporization of the liquid fuel
L'	effect heat of vaporization
Le	Liquid fuel Lewis number
Nu	Nusselt number based on droplet diameter
p	r/R
Pe	Peclet number
Pr	Prandtl number
r	radial distance in spherical polar coordinate system

R	droplet radius; also as distance from axis of symmetry
R_o	initial droplet radius
s	Laplace Transform parameter
t	physical time
T	nondimensional temperature
T	nondimensional temperature T after the Laplace Transform
T_w	average streamline temperature within the droplet
T_b	boiling temperature of liquid fuel
T_o	initial droplet temperature
T_s	nondimensional droplet surface temperature
T_∞	ambient temperature
U_1	velocity in the streamwise direction
u	x-component of velocity
v	y-component of velocity
x	cartesian coordinate along droplet surface
X	mole fraction
y	cartesian coordinate normal to droplet surface
Y	mass fraction
Y^*	fraction defined by Equation (6.17)

Greek Symbols

α	thermal diffusivity
β	constant in stagnation point velocity relationship
η	Blasius similarity variable; also azimuthal direction in the spherical polar coordinate

θ	tangential coordinate direction
λ	thermal conductivity
μ	dynamic viscosity
ν	kinematic viscosity
ξ	streamwise coordinate
ψ	stream function
ρ	density
τ	nondimensional time defined by Equation (3.18)
τ'	nondimensional time defined by Equation (3.14)
τ^*	nondimensional time defined by Equation (6.16)
ϕ	dimensionless stream function defined by Equation (3.7)
ϕ_0	value of ϕ at the bounding stream surface of the core

Subscripts

$b\ell$	liquid thermal boundary layer
e	variable evaluated at the edge of the gas-phase boundary layer
F	variable pertains to fuel vapor
g	gas-phase variable
ℓ	liquid-phase variable
s	variable evaluated at droplet surface

(Other symbols are defined in the text.)

VOL. I. FUEL DROPLET VAPORIZATION THEORY

CHAPTER 1

INTRODUCTION

1.1. Importance of Droplet Vaporization Study

The combustion of liquid fuel sprays is of substantial practical importance. It is involved in many combustion systems such as liquid rocket engines, after burners, carburetors, and ramjets. The temperature inside a combustion chamber is typically high. The liquid fuel droplets injected inside the chamber undergo vaporization and subsequently combustion. To improve the performance of engines using spray injections, studies on the vaporization and combustion of the spray are of vital importance. A prerequisite for any understanding of spray combustion and its application to the design of efficient combustion systems is the knowledge of the physics governing the rate of droplet vaporization. However, the physical phenomena of evaporating and combusting sprays is extremely complicated and modeling it is very difficult. Alternatively, the behaviors of individual droplets can serve as fundamental inputs to the spray analysis. In particular, an understanding of the vaporization and kinematic behavior of a single, isolated droplet in an infinite expanse of gas would be useful for gaining insights on the mechanisms governing complex heterogeneous spray combustion systems.

1.2. Objective of this thesis

The problem of droplet vaporization in a hot convective gaseous environment, taking into account the liquid-phase internal circulation and unsteady droplet heating, is the major concern of this thesis. Although the process of droplet vaporization and combustion in a combustor is typically very fast, the process is essentially unsteady in the frame of reference of a

liquid droplet. The initially cold droplet heats up in time and decreases in radius as it simultaneously vaporizes. In addition, the gas-phase convection leads to internal liquid motion which is important in heat and mass diffusion within the droplet. The spherically symmetric situation will also be significantly modified.

As will be discussed in the next section, the models existing in the literature are either oversimplified and inadequate for any realistic analysis or too complicated to be useful in a complete spray vaporization calculation. In view of that, the main objective is to develop an algorithm for the droplet vaporization which is simple enough to be feasibly incorporated into a complete combustion analysis and yet will also account for the important physics such as liquid-phase internal circulation, unsteady droplet heating and axisymmetric gas-phase convection. The single-component droplet and the multicomponent droplet will both be considered. In addition, the problem of time varying free-stream velocity and the effect of varying ambient temperature will also be examined.

1.3. Approach Adopted in this Research

Recently, the convective transient vaporization problem has been thoroughly studied by Prakash and Sirignano [1,2] for a single-component fuel droplet. Their analysis has also been extended to the multicomponent fuel droplet case by Lara-Urbaneja and Sirignano [3]. The model used in these studies accounts for the important physics stated earlier. Although the model is quite detailed, the algorithm is too complicated and computer time consuming to be incorporated in a full analysis of spray vaporization in a combustor. The present research focuses on simplifying these studies and attempts to develop a simpler algorithm which requires less computation and is more suitable for complete spray combustion analysis.

1.4. Organization of Thesis

A brief literature review on single droplet vaporization theories is given in the next chapter. The unsteady liquid-phase analysis is presented in Chapter 3 which is followed by the quasi-steady gas-phase analysis in Chapter 4. The coupling of the gas-phase solution to the liquid-phase solution is described in Chapter 5. The results of the coupled vaporization problem by using various solution schemes are also reported in that chapter. In Chapter 6, a brief review of multicomponent droplet vaporization studies is given which is followed by an extension of the single-component droplet analysis. Again the results of the coupled vaporization problem for a bicomponent droplet by using different solution schemes are given. In addition, the effects of the various liquid-phase models on the vaporization behaviors of a bicomponent droplet are also examined. The use of the different liquid-phase models in a spray vaporization situation is described in Chapter 7. A transient one-dimensional flow of an air-fuel droplet mixture in an open tube is considered. The effects of the different droplet models on the vaporization characteristics are reported in Chapter 8. In Chapter 9, the results of the present model as well as several other models are compared with the available experimental data. Finally, conclusions, discussions and suggestions for future studies are given in Chapter 10.

CHAPTER 2

LITERATURE REVIEWS ON SINGLE DROPLET VAPORIZATION THEORIES

There has been a great deal of work, both theoretical and experimental, on the problem of a vaporizing fuel droplet. Extensive reviews have been given by Williams [4], Faeth [5], Sirignano and Law [6], Sirignano [7] and Law [8]. Some of the literature relevant to the present study will be reviewed in this section.

The theory of fuel droplet vaporization and spray combustion has been under development for several decades. During recent years, as new and heavier fuels become common, droplet vaporization in a liquid-fueled combustor becomes more significant as a rate-controlling factor. The problem of droplet vaporization has come to receive a large amount of attention. Basically, the existing literature on single droplet vaporization can be classified into two major categories: spherically-symmetric and axisymmetric. The different models in these two categories are discussed below.

2.1. Spherically Symmetric Models

2.1.1. d^2 Law Model

The most notable earlier work on droplet vaporization is by Godsave [9]. In that study, a quasi-steady spherically-symmetric model was used. The droplet temperature was assumed to be uniform and remained constant at its wet-bulb value. The properties in both the gas and liquid phases were assumed to be constant, together with Lewis number equal to unity. At the gas-liquid interface, it was assumed that the fuel vapor mass fraction was a

function of the surface temperature given by some equilibrium vapor pressure equation such as the Clausius-Clapeyron relation. This theory gives the classic d^2 -law and is the simplest possible model describing droplet vaporization. It should be noted that this model neglects the liquid-phase heat and mass transfer and is basically a gas-phase model. It does not consider some of the important physics and only yields a crude estimate of the droplet vaporization rate.

Some of the resulting relationships are given below:

$$\frac{m}{4\pi R \rho_g D} = \ln(1+B) \quad (2.1)$$

$$B = \frac{C_{pg} (T_g - T_s)}{L} = \frac{Y_{fs}}{1 - Y_{fs}} \quad (2.2)$$

where m is the fuel mass vaporization rate, B is the Spalding Transfer number, L is the latent heat of fuel and Y_{fs} is the fuel vapor mass fraction at the interface. Subscripts g and s denote gas phase and droplet surface, respectively.

Note that $Y_{fs} = Y_{fs}(T_s)$ is a function of surface temperature only. Therefore T_s and B can be determined by Equation (2.2) and subsequently can be obtained through Equation (2.1). For a given ambient condition, T_s and B are fixed in this model, Equation (2.1) can be written as

$$\frac{dR^2}{dt} = k = \text{constant} \quad (2.3)$$

which says that the radius squared (proportional to the droplet surface area)

decreases linearly in time and hence this model is referred to as d^2 -law model in the literature.

2.1.2. Infinite Conductivity Model

In a combustor, the droplet is initially cold and heats up with time. The initial transient droplet heating period has only recently been given attention. Law [10] studied droplet combustion with rapid internal mixing where droplet temperature is spatially uniform but varying with time. Sample calculations were performed for heptane droplets burning in the standard atmosphere with ambient temperature and pressure respectively equal to 300°K and 1 atmosphere. It was found that droplet heating is a significant cause of the unsteadiness of droplet combustion and should be taken into account in any realistic analysis of unsteady droplet combustion phenomena. Basically, this model is the same as the d^2 -law model except that the constant liquid-phase temperature assumption is relaxed and is replaced by a uniform but time-varying temperature inside the droplet. The gas-phase model remains spherically symmetric and quasi-steady.

Some authors believed that this uniform temperature limit is related to the rapid internal liquid circulation limit and hence is referred to as rapid mixing model. Sirignano [11] showed that even in the limit of high vortex strength, the internal liquid circulation can only reduce the characteristic length scale for diffusion by an order of magnitude. The rapid mixing limit can never exist. Rather, it would be conceptually more correct to think that the uniform temperature limit results from the infinite conductivity limit. Hence it is more appropriate to call it an infinite-conductivity model.

Equations (2.1) and (2.2) remain the same except that L is replaced by

$$L + \frac{1}{m} \left(\frac{4}{3} \pi R^3 \rho_\ell c_{p\ell} \right) \frac{dT_\ell}{dt}$$

The additional term accounts for the transient liquid droplet heating. Subscript ℓ denotes the liquid phase.

2.1.3. Conduction Limit Model

When the internal liquid motion is not significant, heat transfer inside the droplet will be controlled by thermal diffusion only. This will be a reasonable model for the stagnant case and represents the slowest heat transfer limit.

The liquid-phase temperature variation is governed by the well known heat diffusion equation,

$$\frac{\partial T_\ell}{\partial t} = \frac{\alpha_\ell}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) \quad (2.4)$$

with the initial and boundary conditions

$$(i) \text{ at } t = 0; T(r, t) = T_0(r)$$

$$(ii) \text{ at } r = 0; \frac{\partial T(r, t)}{\partial r} = 0$$

$$(iii) \text{ at } r = R_s(t); k_\ell \frac{\partial T(r, t)}{\partial r} = q_\ell(t) \quad (2.5)$$

where $T_0(r)$ is the initial temperature distribution and $q_\ell(t)$ is the liquid-phase heat flux at the droplet surface.

Equations (2.1) and (2.2) remain essentially the same except that L is replaced by

$$L + \frac{1}{m} \left(4\pi R^2 k_\ell \left. \frac{\partial T}{\partial r} \right|_s \right).$$

The additional term accounts for the liquid-phase heat flux at the surface.

Since the droplet is vaporizing, the diffusion field has a moving boundary. Obviously this model is more complicated than the infinite conductivity limit model. By using the above formulation, Law and Sirignano [12] studied droplet combustion with droplet heating by conduction alone. Sample calculations were performed for octane droplets burning in the standard atmosphere with ambient temperature and pressure respectively equal to 300°K and 1 atmosphere. The results of the two studies indicate that droplet heating is the dominant heat utilization mode for the initial 20-30% of the droplet lifetime and is a significant cause of the unsteadiness of droplet combustion. The droplet temperature differs substantially in magnitude in the two limits for most of the droplet lifetime. With the rapid mixing limit the droplet temperature reaches a constant value in an unsteady period of about 10 to 20% of droplet lifetime. While in the more realistic conduction limit, it takes a substantially longer time for the droplet center temperature to reach the almost constant surface temperature. If detailed temperature distribution within a droplet is crucial, then unsteadiness persists throughout the droplet lifetime. It is expected that heavier fuels will have longer transient periods.

Hubbard *et al.* [13] numerically solved the complete unsteady gas- and liquid-phase heat and mass conservation equations considering variable properties. Sample calculations for octane droplets initially at 300°K

evaporating into air at temperatures and pressures in the ranges 600-2000°K and 1-10 atmospheres, respectively were reported. They also found, for the cases studied, that overall quasi-steadiness exists in about 20-30% of the droplet lifetime and the transient behavior is due to the droplet heating. The gas-phase quasi-steadiness assumption was also proved to be a proper approximation.

2.2. Droplet Vaporization with Convective Effects

2.2.1. Ranz-Marshall Model

The studies discussed so far are based on the model of spherical symmetry. In reality, the practical problem of droplet vaporization in a spray involves a convective situation in which there is a relative gas-droplet velocity. Many investigators [4,5] suggested empirical correlations for vaporization rate in a convective field as a correction to the spherical symmetric case. The typical form of correlation is $m_{\text{convection}} = m_{\text{spherical}} F(\text{Re}, \text{Pr})$ where $F(\text{Re}, \text{Pr})$ is the correction factor. In the present study, the Ranz-Marshall correlation is examined, for which the factor $F(\text{Re}, \text{Pr})$ is given by

$$F(\text{Re}, \text{Pr}) = 1 + 0.3 \text{Re}^{1/2} \text{Pr}^{1/3} \quad (2.6)$$

Although this type of correlations is very simple, there is really very little theoretical justification for them. Moreover, these correlations are based on experiments conducted under quasi-steady conditions. As mentioned before, there is a transient droplet heating stage and during that period the quasi-steadiness assumption is invalid. Indeed Sirignano [11] showed, through theoretical analysis, that a correlation of Ranz-Marshall type cannot satisfactorily predict the vaporization rate.

2.2.2. Prakash and Sirignano's Axisymmetric Model

Recently, Prakash and Sirignano [1,2], studied the problem of transient liquid droplet vaporization in a hot convective environment. They first [1] studied liquid internal circulation and droplet heating and later [2] developed a gas-phase boundary layer analysis and coupled it to the previous liquid-phase analysis. Basically, they used a two-dimensional axisymmetric model and divided the problem into several physical regions as shown in Figure 2.1. These regions were: outer inviscid gas flow, gas-phase boundary layer, liquid-phase boundary layer, internal liquid wake and inviscid liquid core. Because of the relatively high Reynolds number and high Peclet number, the boundary layer approximation was used in their analysis for both the momentum and the energy transfers in both the gas and the liquid phases. The outer inviscid gas flow was treated as steady potential flow around a sphere with no flow separation. The gas-phase and liquid-phase boundary layers were both treated as quasi-steady for both momentum and energy transfer, while for the liquid core, the momentum transfer was treated as quasi-steady and the energy transfer was considered transient. In the liquid-phase analysis, the liquid motion in the core was inviscid with the viscous effects confined to the liquid boundary layer. The core motion was governed by Hill's spherical vortex and the vortex strength was determined as a function of the shear stress along the droplet surface.

Due to the small characteristic time of particle circulation along the streamline in the core, the temperature along each streamline was assumed to be uniform. Thus, the heat flux occurred normal to the streamlines. As a result, an orthogonal streamline coordinate system was used and the problem was simplified to a one-dimensional problem.

For the viscous boundary layer, which exists due to unmatched shear stress

at the interface, the velocity field was shown to be perturbed only slightly. The momentum boundary layer equation was therefore linearized and classical diffusion equation was obtained through some variable transformations. In addition, the vorticity was shown to be convected passively without diffusion as it travels in the region near the stagnation point, through the internal wake, turns to near the front stagnation point and re-enters the boundary layer. This provided a matching condition for the boundary layer equation along the front and rear regions. The other boundary conditions were: (1) the continuity of the tangential forces in the θ direction, i.e., the shear stress in the gas side of the interface is balanced by the liquid-phase shear stress. The shear stress distribution was obtained from the gas-phase solution which resulted in a coupling between the gas- and liquid-phases; (2) at the edge with the inviscid core, the boundary layer solution was required to match smoothly to the Hill's vortex solution in the core.

The quasi-steady analysis of the thermal boundary layer was quite analogous to the viscous boundary layer analysis. The thermal boundary layer equation was linearized and through some variable transformations classical diffusion equation was obtained. It was shown that there is negligible diffusion of heat in the turning region near the rear stagnation point and in the internal wake. The temperature gradient is convected without sensible diffusion through these regions to re-enter the thermal boundary layer. As in the viscous boundary layer case, this provided a matching condition for the boundary layer equation. The other boundary conditions were (1) at the interface, the liquid-phase heat flux is obtained from the gas phase boundary layer solution and (2) at the thermal core matching region, the temperature gradient is uniform but time dependent.

For the quasi-steady gas-phase analysis, boundary layer equations were

derived. An integral approach, which was an extension of the Karman-Polhausen method, was used, and non-linear coupled ordinary differential equations were obtained. These gas-phase equations were coupled to the liquid-phase equations through the interfacial constraints to be satisfied.

The problem was solved by employing the finite difference scheme in conjunction with matching the gas-phase and liquid-phase solution at the interface. The gas-phase solution involved a system of ordinary differential equations and the liquid-phase solution involved parabolic type partial differential equation as well as Fredholm type integral equation. The solution scheme required iteration between the gas-phase solution and the liquid-phase solution at each time step. Thus, even though the model is quite detailed, the algorithm is too cumbersome and computer time consuming to be included in a complete spray vaporization analysis.

CHAPTER 3

LIQUID-PHASE ANALYSIS

3.1. Removal of the Thermal Boundary Layer

3.1.1. Introduction

It was shown in Prakash and Sirignano's analysis [1,2] that the liquid motion is quasi-steady in the limit of large Reynolds number and consists of a Hill's spherical vortex near the droplet surface and an inviscid internal wake near the axis of symmetry. Similarly, there is a thin thermal boundary layer near the droplet surface. The analysis of the thermal boundary layer is similar to that of the viscous boundary layer and there is coupling to the thermal core in the matching region. In the turning region near the rear stagnation point and in the internal wake, there is negligible diffusion of heat and that the temperature gradient is convected without diffusion through this region to re-enter the thermal boundary layer. In that study, the thermal boundary layer allows for the heat flux to adjust from two-dimensional behavior along the droplet surface to one-dimensional behavior along the boundary layer and thermal core matching region.

Although the non-dimensional temperature change across the thermal boundary layer is of the order of $Pe^{1/2}$ and the neglect of the thermal boundary layer would cause only a small error of the same order in determining the temperature field in the droplet, such a coupling is essential in the ultimate problem of droplet vaporization because the fuel vapor fraction and hence the vaporization rate, which in turn determines the heat flux, depends exponentially on the surface temperature. There were no calculations made in that study to estimate the error introduced if the thermal boundary

layer temperature had been represented as one-dimensional. Furthermore, the thermal boundary layer was treated as quasi-steady and the thermal inertia term was ignored. Although the thermal boundary layer is thin, it may still have a significant volume and mass due to its location near the surface. Therefore, the thermal inertia term cannot always be disregarded and the quasi-steadiness assumption can be invalid.

In this section, the importance of the two-dimensional representation of the thermal boundary layer as well as the quasi-steadiness assumption are examined. They are described below.

3.1.2. Importance of the Two-Dimensional Representation of the Thermal Boundary Layer and the Quasi-Steadiness Assumption

To set aside certain complications, the non-vaporizing liquid phase problem, decoupled from the gas phase, is considered first. The surface heat flux is specified in a boundary condition with a profile similar to those obtained in [2] and is time invariant.

In [2], the energy balance at the droplet surface for the vaporizing droplet case was expressed as (Equation (17) in [2])

$$\left(\frac{\lambda}{C_p} \frac{\partial h}{\partial y} \right)_{s,g} = (\rho v)_s L + \left(\lambda \frac{\partial T}{\partial y} \right)_{s,l} \quad (3.1)$$

where subscript s refers to the droplet surface and subscripts g and l refer to the gas phase and liquid phase respectively. L is the latent heat of vaporization. The term on the left-hand side represents the gas-phase heat flux at the droplet surface. The terms on the right hand side correspond to the latent heat of vaporization and the liquid phase heat flux respectively and $(\rho v)_s$ corresponds to the vaporization mass flux at the droplet surface.

In the non-vaporizing case, $(\rho v)_s = 0$ and Equation (3.1) simplifies to:

$$\left(\frac{\lambda}{C_p} \frac{\partial h}{\partial y} \right)_{s,g} = \left(\lambda \frac{\partial T}{\partial y} \right)_{s,l} \quad (3.2)$$

That is, all the heat from the gas phase goes to heat up the liquid inside the droplet. For a given thermal boundary layer thickness, the mass outside the thermal core is estimated and a thermal inertia correction term based on the increase of the average boundary layer temperature during the previous time interval is computed. It is given by

$$(\rho_l \Delta V C_{pl}) \left(\frac{\Delta T}{\Delta t} \right)_{bl} \quad (3.3)$$

where ΔV is the combined volume of the liquid in the thermal layer and in the internal wake and $(\Delta T/\Delta t)_{bl}$ is the time rate of increase of the average boundary layer temperature. Dividing by the droplet surface area, the thermal inertia correction term is put into the dimensions of a heat flux given by

$$\left(\frac{\rho_l \Delta V C_{pl}}{4\pi R^2} \right) \left(\frac{\Delta T}{\Delta t} \right)_{bl} \quad (3.4)$$

It is then added to the right hand side of Equation (3.2) to compensate for the liquid boundary layer thermal inertia which was neglected in the quasi-steady thermal boundary layer formulation. Therefore, Equation (3.2) becomes:

$$\left(\frac{\lambda}{C_p} \frac{\partial h}{\partial y} \right)_{s,g} = \left(\lambda \frac{\partial T}{\partial y} \right)_{s,l} + \left(\frac{\rho_l \Delta V C_{pl}}{4\pi R^2} \right) \left(\frac{\Delta T}{\Delta t} \right)_{bl} \quad (3.5)$$

This thermal inertia correction term, although a crude estimation, is believed to be sufficiently accurate for examining the thermal boundary layer

steadiness assumption. A more accurate study would have a thermal inertia term placed directly into the governing partial differential equation for the thermal boundary layer and involve a time-dependent boundary layer solution coupled to the transient thermal core solution.

To study the importance of the thermal boundary layer, several different locations for matching boundary layer and core solutions are examined including the extreme case without the two-dimensional representation of the thermal boundary layer. In the last case, the whole droplet is treated as a thermal core throughout. Note that while the thermal boundary layer formulation is two-dimensional, the thermal core formulation is one-dimensional. The simplification of the thermal boundary layer representation would simplify the problem from a two-dimensional to a one-dimensional situation.

The liquid fuel considered in the computation is n-hexane and the initial conditions as well as the physical properties are the same as in [2]. The results are summarized below.

3.1.3. Results and Discussions

The results are shown in Figures 3.1 to 3.3. In these figures, symbols are attached at both ends of the curves for identification. The non-dimensional time, τ , and the non-dimensional stream function, ϕ , are as defined in [2]. It should be mentioned that in the case of the core solution, the thermal boundary layer is removed and the thermal core extends to the droplet surface. Due to the logarithmic singularity of the function g_1 (defined in [2]) at the surface, the core solutions shown in the figures are actually calculated up to $\phi = 0.99$. It is quite close to the droplet surface and the estimated resulting errors are considered to be acceptable for the present study. In reality, the

boundary layer profile decays exponentially with the decreasing ϕ ; for our purposes, the boundary layer thickness is defined as the value of $1-\phi$ determined by the point where the boundary layer solution and the core solution are matched. In the figures, the boundary layer in case number 3 is of the same thickness as that used in [2] and is about twice as thick as the boundary layer in case number 2 which in turn is about twice as thick as the boundary layer in case number 1.

The results for the core temperature distribution are shown in Figure 3.1. The results for the core solution and for those with thermal inertia correction are in close agreement. The slightly higher temperature of the core solution at the later time may be in part due to the crude correction and in part due to the fact that $\phi = 0.99$ instead of $\phi = 1.00$ is used as the boundary in the core solution. On the other hand, the temperatures for those with no thermal inertia correction are all considerably higher and depend strongly on the boundary layer thickness. While the effect of the thermal boundary layer is to smooth the surface heat flux variation, the total heat energy into the droplet is preserved. The differences in the core temperatures are therefore due to the neglect of the thermal inertia term in the thermal boundary layer.

The results for the surface temperature are shown in Figure 3.2. Again the surface temperatures for those without thermal inertia correction are higher. The average variation in temperature is quite close to those with thermal inertia correction. The lower temperature obtained for those with thermal inertia correction as compared to the core solution is believed to result from over-correction. The heat flux in the thermal boundary layer has not been corrected gradually from the droplet surface to the thermal core matching region, but rather it has been corrected completely at the droplet surface. That is, the thermal inertia of the boundary layer has been modelled by adding

a term in the energy balance at the surface that is the product of the mass in the layer and the time rate of change of the average specific enthalpy in the layer. This correction scheme indirectly affects the core heat flux and hence the core temperature, and results in lower surface temperatures. This correction will be smallest on the thinnest boundary layer and the core solutions are quite close to those of boundary layer case number 1 and can be considered to be reasonable average surface temperature approximation.

The results for the fuel vapor mass fraction along the droplet surface are plotted in Figure 3.3. They are evaluated at the droplet surface temperature based upon a Clausius-Clapeyron equilibrium assumption and are therefore subjected to the same overcorrection error mentioned earlier. The percentage variation in the mass fraction is larger at the early time instant and decreases with time as the droplet temperature increases. It is about 15% at $\tau=0.01$ and about 7% at $\tau=0.03$. It should be noted that in the vaporizing case, it was found in [2] that the vaporization rate is small during the initial droplet heat-up period and increases gradually until it finally becomes vaporization dominated. Therefore, if the surface mass fraction is represented by an average value, i.e. in the case when the thermal boundary layer is eliminated, the relatively larger error in the mass fraction in the early period will not lead to large error in the overall vaporization rate.

The results of this study show that, unless the thermal boundary layer is very thin (very large Peclet numbers), the thermal inertia term is important and the quasi-steadiness assumption is invalid. The results also tend to suggest that the elimination of the thermal boundary layer and the assumption that the core is valid up to the droplet surface may still give solutions with acceptable degrees of accuracy. To verify completely the above observation, a more vigorous study which involves the coupled droplet vaporization problem with

the addition of a thermal inertia term in the liquid-phase thermal boundary layer equation would be useful.

One normally thinks of a boundary layer as a region across which a variable changes rapidly. For the cases of interest with vaporizing fuel droplets in high temperature gaseous environments, the thermal boundary layer beneath the liquid surface is not a region where temperature gradients normal to the stream surfaces are much larger than in the core region; rather, the core and the layer gradients are of the same order of magnitude and the temperature variation in the layer is not more severe than in the core. A greater degree of variation occurs in the streamwise gradient of the temperature. That gradient is zero in the core region and varies through the thin boundary layer with the largest value at the surface. For this reason, the boundary layer in the liquid is a region of adjustment between the one-dimensional core behavior and the two-dimensional gas-phase behavior.

Even though a large Peclet number exists, the energy equation for the thermal layer does not take the limiting form with a primary balance of a convective term with the diffusive term. In particular, the time-derivative term is at least as important as the other terms. The neglect of the convective term is not a bad approximation and allows the reduction of the problem from two-dimensionality to one-dimensionality.

Therefore, through the evaluation of the boundary, it is seen that, instead of a two-dimensional quasi-steady representation, a one-dimensional unsteady representation can be made.

3.1.4. Summary

The importance of liquid thermal boundary layer in the transient heating of a liquid droplet with internal circulation is examined. The thermal boundary layer quasi-steadiness assumption is also studied. The results show that, unless the thermal boundary layer is extremely thin (extremely large Peclet numbers), the thermal inertia term is important and the quasi-steadiness assumption is invalid. The results also tend to suggest that the elimination of the thermal boundary layer may still give solutions with acceptable degree of accuracy.

3.2. Unsteady Thermal Core Analysis

3.2.1. Introduction

With the elimination of the thermal boundary layer and the assumption that the thermal core solution is valid up to the droplet surface, the thermal core solution is examined in this section. The energy equation for the thermal core is simplified and series solution for both the constant temperature boundary condition and the constant temperature gradient boundary condition cases are obtained. The results are in reasonably close agreement with the finite-difference solutions of the unsimplified equation.

Because of the linear nature of the problem, the series solutions can be superimposed to generate solutions for the time-varying boundary condition cases. In the non-vaporizing droplet case, the coupled gas-phase and liquid-phase problem is examined. With the legitimate assumption of constant Nusselt number and utilizing the series solution, solution for the droplet surface temperature in the form of a linear Volterra-type integral equation is obtained. The application of the series solution to the vaporizing droplet case is also examined and is presented in the coupled solution section following the section on the gas-phase analysis.

3.2.2. Thermal Core Solution

In Prakash and Sirignano's analysis [1,2], the droplet core heating was shown to be essentially unsteady and normal to the closed streamlines because of a very short residence and circulation time along a streamline compared to the droplet lifetime. Therefore, the orthogonal streamline coordinates were used for the energy equation in the droplet core. In the orthogonal streamline coordinate system (ξ, ψ, η) (see Figure 3.4), the scale factors are given by

$$h_{\xi} = A r^5 \cos^5 \theta / 2 U_1$$

$$h_{\psi} = 1/(r U_1 \sin \theta) \quad (3.6)$$

$$h_{\eta} = r \sin \theta$$

A non-dimensional stream function was defined such that its value is zero at the vortex center and unity at the droplet surface. Thus,

$$\phi = 8\psi/AR^4 = 1 - 4p^2 (1-p^2) \sin^2 \theta \quad (3.7)$$

where A is the strength of the Hill's vortex and $p = r/R$. Defining,

$$g_1(\phi) = \frac{AR}{8} \oint h_{\xi} h_{\psi} h_{\eta} d\xi \quad (3.8)$$

$$g_2(\phi) = \frac{8}{AR^5} \oint \frac{h_{\eta}}{h_{\psi}} h_{\xi} d\xi \quad (3.9)$$

The energy equation valid in the core was found to be

$$\frac{\partial T}{\partial \tau'} = a(\tau', \phi) \frac{\partial^2 T}{\partial \phi^2} + b(\tau', \phi) \frac{\partial T}{\partial \phi} \quad (3.10)$$

where

$$a(\tau', \phi) = \frac{R_0^2}{R^2} \frac{g_2(\phi)}{g_1(\phi)} \quad (3.11)$$

$$b(\tau', \phi) = \frac{1}{g_1(\phi)} \frac{R_0^2}{R^2} \frac{dg_2(\phi)}{d\phi} + \frac{3}{g_1(\phi)R} \frac{dR}{d\tau'} \int_0^\phi g_1(\phi) d\phi \quad (3.12)$$

$$T = \frac{T_{av} - T_0}{T_b - T_0} \quad (3.13)$$

$$\tau' = at/R_0^2 \quad (3.14)$$

The initial and boundary conditions were:

$$(i) \text{ at } \tau' = 0, T = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial T}{\partial \tau'} = b(\tau', \phi) \frac{\partial T}{\partial \phi}$$

$$(iii) \text{ at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = q_1(\tau') \quad (3.15)$$

The boundary $\phi = \phi_0$ corresponds to the outer boundary of the core near the droplet surface. In the boundary condition (iii) above, the temperature gradient

$q_1(\tau')$ was obtained by requiring the continuity of heat flux in the interfacing region of the thermal boundary layer and the thermal core. Equation (3.10) was solved numerically using a Crank-Nicholson scheme and the solution was marched forward in time. The details of the formulation is given in [16].

To seek a simpler solution to Equation (3.10), the functions $g_1(\phi)$ and $g_2(\phi)$ are examined in this study. They are evaluated numerically and are shown graphically in Figure 3.5. In most regions, the function $g_1(\phi)$ varies slowly with ϕ while the function $g_2(\phi)$ varies linearly with ϕ . Approximating them by

$$g_1(\phi) = b_0; \quad g_2(\phi) = b_1\phi \quad (3.16)$$

where b_0 and b_1 are constants, Equation (3.10) simplifies to

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + [1 + C(\tau)\phi] \frac{\partial T}{\partial \phi} \quad (3.17)$$

where

$$d\tau = \frac{b_1}{b_0} \frac{R_0^2}{R^2} dr' \quad (3.18)$$

and

$$C(\tau) = 2 \left(\frac{R_0}{R} \right)^{3/2} \frac{d}{dr} \left(\frac{R}{R_0} \right)^{3/2} \quad (3.19)$$

The function $C(\tau)$ relates to the droplet vaporization rate and is coupled to the gas-phase solution. In general, $C(\tau)$, would be a function of τ . Nevertheless, the simple case where $C(\tau)$ equals a constant C_0 , is examined first, followed by the more general time-varying C case. For $C = C_0$,

Equations (3.17) and the associated initial and boundary conditions (3.15) become

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + (1 + C_0 \phi) \frac{\partial T}{\partial \phi} \quad (3.20)$$

and

$$(i) \text{ at } \tau = 0, T = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$$

$$(iii) \text{ at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = q_2(\tau) \quad (3.21)$$

By taking the Laplace Transform on τ , Equation (3.20) and the boundary conditions (3.21) become

$$\phi \frac{d^2 T(s, \phi)}{d\phi^2} + (1 + C_0 \phi) \frac{dT(s, \phi)}{d\phi} - sT(s, \phi) = 0 \quad (3.22)$$

$$(i) \text{ at } \phi = 0, \frac{dT(s, 0)}{d\phi}, -sT(s, 0)$$

$$(ii) \text{ at } \phi = \phi_0, \frac{dT(s, \phi_0)}{d\phi} = q_2(s) \quad (3.23)$$

The solution for the unity temperature gradient boundary case where $q_2(s) = 1/s$ is given by

$$T(s, \phi) = F(s, C_0, \phi) / s G(s, C_0, \phi_0) \quad (3.24)$$

where

$$F(s, C_0, \phi) = 1 + \sum_{k=1}^{\infty} \frac{s(s-C_0) \dots [s-(k-1)C_0]}{(k!)^2} \phi^k \quad (3.25)$$

and

$$G(s, C_0, \phi) = \frac{\partial F}{\partial \phi}(s, C_0, \phi) \quad (3.26)$$

and by means of the Inversion Integral Technique

$$T(\tau, \phi) = \frac{\tau + F_s(0, C_0, \phi)}{G_s(0, C_0, \phi_0)} - \frac{1}{2} \frac{G_{ss}(0, C_0, \phi_0)}{G_s^2(0, C_0, \phi_0)} \quad (3.27)$$

$$+ \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_0, \phi)}{\lambda_n G_s(\lambda_n, C_0, \phi_0)} \exp(\lambda_n \tau)$$

where the λ_n 's are the roots of $G(\lambda_n, C_0, \phi_0) = 0$. In Equation (3.27),

$$F_s(0, C_0, \phi) = \frac{\partial}{\partial s} F(s, C_0, \phi) \Big|_{s=0} \quad (3.28)$$

$$G_s(0, C_0, \phi) = \frac{\partial}{\partial s} G(s, C_0, \phi) \Big|_{s=0} \quad (3.29)$$

$$G_{ss}(O, C_O, \phi) = \frac{\partial^2}{\partial s^2} G(s, C_O, \phi) \Big|_{s=0} \quad (3.30)$$

For the unity temperature case, i.e. $T(\tau, \phi) = 1$, it can be shown that the temperature distribution is given by

$$T(\tau, \phi) = 1 + \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_O, \phi)}{\lambda_n F_s(\lambda_n, C_O, \phi_O)} \exp(\lambda_n \tau) \quad (3.31)$$

where the λ_n 's are the roots of $F(\lambda_n, C_O, \phi_O) = 0$. The details of the derivation are given in Appendix E. For the non-vaporizing case, $C=0$, (see Equation 3.19) the solutions can be expressed in terms of Bessel functions. For the unity temperature gradient case,

$$T(\tau, \phi) = \phi - \frac{\phi_O}{2} + \tau - 4\phi \sum_{n=1}^{\infty} \frac{J_0(\lambda_n (\phi/\phi_O)^{1/2})}{\lambda_n^2 J_0(\lambda_n)} \exp\left(-\frac{\lambda_n^2}{4\phi_O} \tau\right) \quad (3.32)$$

where $J_1(\lambda_n) = 0$. For the unity temperature case,

$$T(\tau, \phi) = 1 - \sum_{n=1}^{\infty} \frac{2}{\lambda_n} \frac{J_0(\lambda_n (\phi/\phi_O)^{1/2})}{J_1(\lambda_n)} \exp\left(-\frac{\lambda_n^2}{4\phi_O} \tau\right) \quad (3.33)$$

where $J_0(\lambda_n) = 0$.

The details of the derivation are summarized in Appendix D. For the time dependent C case, $C = C(\tau)$; by the following change of variables:

$$V(\tau, \phi) = T(\tau, \phi) \operatorname{sech}\left(\frac{k\tau}{2}\right) \exp\left(\frac{-k\phi}{2} \tanh\left(\frac{k\tau}{2}\right)\right) \quad (3.34)$$

Equations (3.17) and (3.21) are transformed to

$$\frac{\partial V}{\partial \tau} = \frac{\partial^2 V}{\partial \phi^2} + \frac{\partial V}{\partial \phi} - \frac{k^2}{4} \phi V \quad (3.35)$$

(i) at $\tau = 0$, $V = 0$

$$(ii) \text{ at } \phi = 0, \quad \frac{\partial V}{\partial \phi} = \frac{\partial V}{\partial \tau}$$

$$(iii) \text{ at } \phi = \phi_0, \quad \frac{\partial V}{\partial \phi} = q_2(\tau) \operatorname{sech}\left(\frac{k\tau}{2}\right) \exp\left(\frac{C\phi_0}{2}\right) + \frac{C}{2} V \quad (3.36)$$

where $C(\tau)$ in this case is approximated by

$$C = -k \tanh(k\tau/2) \quad (3.37)$$

and the constant k is determined such that Equation (3.37) provides the best fit to a given function C . The details of the derivation are reported in Appendix F. Later, we will demonstrate that acceptable fits can be established. The solution for V is given by

$$\begin{aligned} V(\tau, \phi) = & u(0, \phi) \left[f(\tau) + \frac{1}{2} C(\tau) V(\tau, \phi_0) \right] + \int_0^\tau \frac{\partial u}{\partial \tau}(\tau-x, \phi) f(x) dx \\ & + \frac{1}{2} \int_0^\tau C(x) V(x, \phi_0) \frac{\partial u(\tau-x, \phi)}{\partial \tau} dx \end{aligned} \quad (3.38)$$

and

$$u(\tau, \phi) = \frac{W(0, k, \phi)}{W_\phi(0, k, \phi_0)} + \sum_{n=1}^{\infty} \frac{W(\lambda_n, k, \phi)}{\lambda_n W_{s\phi}(\lambda_n, k, \phi_0)} \exp(\lambda_n \tau) \quad (3.39)$$

where the λ_n 's are the roots of $W_\phi(\lambda_n, k, \phi_0) = 0$.

In Equations (3.38) and (3.39) above,

$$W(s, k, \phi) = \sum_{n=0}^{\infty} A_n \phi^n \quad (3.40)$$

where

$$A_0 = 1, A_1 = s \text{ and } A_{n+2} = \frac{sA_{n+1} + (k^2/4) A_n}{(n+2)^2} \text{ for } n \geq 0.$$

$$W_{\phi}(0, k, \phi_0) = \frac{\partial W(s, k, \phi_0)}{\partial \phi} \Big|_{s=0} \quad (3.41)$$

$$W_{s\phi}(\lambda_n, k, \phi_0) = \frac{\partial^2 W(s, k, \phi_0)}{\partial \phi \partial s} \Big|_{s=0} \quad (3.42)$$

and

$$f(\tau) = q_2(\tau) \operatorname{sech}(k\tau/2) \exp\left(-\frac{k\phi_0}{2} \tanh\left(\frac{k\tau}{2}\right)\right) \quad (3.43)$$

For the temperature boundary condition case, i.e., $T(\tau, \phi_0) = g(\tau)$, the solution is given by

$$V(\tau, \phi) = w(\tau, \phi)g(0) + \int_0^{\tau} w(\tau-x, \phi) \frac{dh(x)}{dx} dx \quad (3.44)$$

$$w(\tau, \phi) = \frac{W(0, k, \phi)}{W(0, k, \phi_0)} + \sum_{n=1}^{\infty} \frac{W(\lambda_n, k, \phi)}{\lambda_n W_s(\lambda_n, k, \phi_0)} \exp(\lambda_n \tau) \quad (3.45)$$

where the λ_n 's are the roots of $W(\lambda_n, k, \phi_0) = 0$.

In Equation (3.44),

$$h(\tau) = g(\tau) \operatorname{sech}(k\tau/2) \exp(C\phi_0/2) \quad (3.46)$$

The details of the derivation are given in Appendix G.

3.3. Results and Discussion

For the non-vaporizing droplet case, the series solutions given by Equations (3.32) and (3.33) were calculated and the results are shown in Figures 3.6 and 3.7. The finite difference solutions for the unsimplified equation [i.e., Equation (3.10)], were also calculated and are plotted alongside those mentioned previously. The results are in close agreement. The value of ϕ_0 was chosen as 0.99 in all the calculations. Equation (3.20) was also solved by the same finite-difference scheme employed for Equation (3.10) and its solution was identical to the analytical solution, guaranteeing that the finite-difference scheme used does give exact solution. Therefore, the differences in Figures 3.6 and 3.7 result solely from the approximations for g_1 and g_2 given before. Truncation errors and round-off errors contribute negligibly.

In the constant C vaporizing droplet case, a representative value of C_0 was obtained after a brief review of the results obtained in [2]. The series solutions given by Equations (3.27) and (3.31) were then computed and the results for the unity temperature gradient and the unity temperature boundary conditions are shown in Figures 3.8 and 3.9, respectively. As in the non-vaporizing case, the finite-difference solutions for the unsimplified equations [i.e., Equations (3.10)] were calculated and are also plotted alongside the corresponding series solutions. The value of C_0 was chosen to be -0.828. The results for both the unity temperature gradient boundary condition case and the unity temperature case are in reasonably close agreement.

As mentioned earlier, the differences in the figures result solely from the approximations for g_1 and g_2 . A closer agreement between the results of the series solutions of the approximated equation and the finite difference solutions of the unsimplified equation can therefore be expected by improving the approximation for g_1 . It was found that for both the vaporizing droplet case and the non-vaporizing droplet case, series solutions can still be obtained for polynomial approximation of g_1 . A first or second order polynomial approximates g_1 reasonably well and the results were found to be in very good agreement with the finite difference solution. It is obvious that the series solution scheme consumes much less computation time than the finite difference method.

It should be mentioned that the series solutions for both the unity temperature and the unity temperature gradient boundary condition cases can be used to generate solutions for the corresponding time dependent boundary condition cases.

In [1], it was shown that the mathematical equations and procedure for the thermal core are similar to those used by Brignell [14] for the problem of solute extraction from an internally circulating liquid drop. On the arguments that the boundary layer is thin and that the diffusion in the core is the rate controlling process, Brignell could solve the problem of mass transfer from the droplet by neglecting the existence of the boundary layer and solving the diffusion equation for the core. He imposed the droplet surface concentration as the boundary condition for the outer boundary of the core, thus eliminating the coupling between the boundary layer and the core without causing any significant errors in the mass transfer problem. The series solution obtained in the section for the non-vaporizing droplet case with unity temperature boundary condition is therefore applicable to Brignell's solute extraction

problem. The fact that series solution exists for any polynomial approximation of g_1 allows the series solution [i.e., Equation (3.33)] to provide a quick and easy way of obtaining high accuracy approximate solution for the solute extraction problem.

For the time varying C vaporizing droplet case, C is approximated by some exponential functions given by Equation (3.44). The values of C as a function of time obtained from the results in [2] are shown in Figure 3.10 along with the exponential approximations. As indicated in the figure, a reasonable curve fit by Equation (3.37) can indeed be found. The series solution given by Equation (3.44) was calculated for the case of unity temperature boundary condition with $k=1.40$. The results shown in Figure 3.11 are again in reasonable agreement with the finite difference solution of Equation (3.10).

Attempts were made to extend the series solutions of the constant C vaporizing droplet case to the varying C vaporizing droplet case. The solution at any given time is obtained by treating C as constant and computing the corresponding series solutions of the constant C vaporizing droplet case. However, the "constant" value of C is set equal to the value of C evaluated at the given time. Unfortunately, the results of this calculation scheme did not compare well with the finite difference solution (after the initial diffusion period) unless C is varying very slowly.

Similar attempts were also made to extend the constant k series solution to the time varying k case. The solution at any given time is obtained by treating k as constant and computing the corresponding series solution of the constant k case. The "constant" value of k is set equal to the value of k at which the approximation curve intersects the exact C curve at that time instant. The results by using this time dependent k scheme were found to be in acceptable agreement with the finite difference solution.

The solution for the time dependent temperature gradient boundary condition case [i.e., Equation (3.38)] involves Volterra type integral equation with series kernel and appears to be lengthy and requires considerable computation in order to obtain the temperature distribution within the core. But, as mentioned earlier, the final goal is to determine the droplet heating rate and vaporization rate and this requires matching the temperature at the gas-liquid interface. In particular, the coupled gas phase and liquid phase problems must be considered here. However, it may be expected that only the temperature at the outer core boundary is needed for determining the vaporization rate. Actually, we need not know the temperature in the droplet interior to determine the heat flux to the droplet and its vaporization rate. This will reduce the amount of computation required for the integral equation tremendously. That is, the one-dimensional, unsteady partial differential equation in the liquid core could be reduced to a time dependent Volterra equation, thereby eliminating spatial dependence from the problem. In Appendix A, the application of this approach to the case of a non-vaporizing droplet is given. The results, shown in Figure A.1, are in surprisingly good agreement with the more exact finite-difference solution. The application of the series solution to the vaporizing droplet case is also examined. The details are discussed in the overall coupled solution of Chapter 5.

3.4. Summary

The problem of convective diffusion in liquid droplet with internal circulation has been analyzed for both the vaporizing and the non-vaporizing cases. Based on the results of the last section, the liquid thermal boundary layer is eliminated and the core solution is considered to be valid to the droplet surface. This removal of the thermal boundary layer simplifies the problem from a two-dimensional situation to a one-dimensional case. The energy

equation for the thermal core is further simplified and series solution for both the constant temperature boundary condition and the constant temperature gradient boundary condition cases are obtained. The results are in reasonably close agreement with the finite-difference solutions of the unsimplified equation. Because of the linear nature of the problem, the series solutions can be superimposed to generate solutions for the time-varying boundary condition cases. The droplet heating problem can be reduced from a multi-dimensional, time-dependent analysis for the liquid interior temperature to only a time-dependent analysis for the surface temperature. The results are most promising for treating the spray combustion problem in a more simplified and manageable manner.

CHAPTER 4

QUASI-STEADY GAS-PHASE ANALYSIS

4.1. Introduction

This chapter focuses on the heat and mass transfer in the gas-phase and searches for a simpler solution scheme which can be coupled to the simplified liquid-phase solution. Here, the effect of convection is not simply represented as an empirical correction to the spherically symmetric droplet vaporization theory. But rather, an axisymmetric analysis is taken. Following Sirignano's analysis [11], the heat and mass transfer rates in the gas-phase are represented by a suitable average for the stagnation point region and the shoulder region (region around 90° from the stagnation point). This approach reduces the dimensionality of the gas-phase model from two to one and is compatible with the simplified one-dimensional liquid-phase solution. The resulting coupled formulation for the droplet vaporization is described in Chapter 5. The results of the coupled solutions are in good agreement with the results of the more detailed model of Prakash and Sirignano [2]. The details of the simplified gas-phase analysis are given here.

4.2. Gas Phase Analysis

A quasi-steady convective gas-phase analysis which considers the stagnation point region and the shoulder region of a droplet where the shoulder region was approximated as a flat plate with zero pressure gradient was done by Sirignano [11]. It was shown in that study that by using a similarity transformation together with a stream function type simplification the governing continuity and momentum boundary layer equations in both the stagnation point and the flat plate analysis could be put into a form of the well-known Blasius equations, namely

$$\frac{d^3 f}{d\eta^3} + f \frac{d^2 f}{d\eta^2} = 0 \quad (4.1)$$

where the similarity variable η was given by

$$\eta = Ru_e \int_0^y \rho \, dy' / \left(\int_0^x 2 \rho_e \mu_e u_e R^2 \, dx' \right)^{1/2} \quad (4.2)$$

Here x and y were the standard boundary layer coordinates and $y=0$ was the gas-liquid interface. The velocity was given by

$$\frac{u}{u_e} = \frac{df(\eta)}{d\eta} \quad (4.3)$$

It was further shown that by assuming the product $\rho\mu$ to be a function of x only. The vaporization mass flux was given by

$$\rho v \Big|_s = -A f(0)$$

where

$$(2\beta \rho_e \mu_e)^{1/2} \quad \text{for stagnation point}$$

$$A =$$

$$\rho_e \mu_e \left(u_e / 2 \int_0^x \rho_e \mu_e \, dx' \right)^{1/2} \quad \text{for flat plate}$$

(4.4)

The boundary conditions were

$$(i) \quad \text{at } \eta=0, \quad \frac{df}{d\eta} = \frac{u_s}{u_e}$$

$$\begin{aligned}
 \text{(ii) at } \eta = \infty, \frac{df}{d\eta} &= 1 \\
 \text{(iii) at } \eta = 0, \frac{d^2f}{d\eta^2} &= \frac{f(df/d\eta - 1)}{B'} \quad (4.5)
 \end{aligned}$$

Boundary condition (iii) was obtained by considering the energy equation in conjunction with the interface boundary conditions. Here B' was the modified Spalding Transfer number which was defined as

$$B' = \frac{h_e - h_s}{L + 1/(\rho v)_s \lambda_\ell (\partial T / \partial y)_{\ell s}} \quad (4.6)$$

B' was shown to be related to the fuel concentration, Y_{fs} , at the droplet surface by

$$B' = \frac{Y_{fs}}{1 - Y_{fs}} \quad (4.7)$$

Here Y_{fs} was a function of the surface temperature given by some equilibrium vapor pressure equation such as Clausius-Clapeyron equation. Note that it is understood that actually $f(\eta) = f(\eta, B')$ and therefore $f(0) = f(0, B')$. Furthermore, the liquid-phase heat flux was given by

$$\lambda_\ell \left(\frac{\partial T}{\partial y} \right)_{\ell s} = -A f(0) \left[\frac{h_e - h_s}{B'} - L \right] \quad (4.8)$$

By considering x to be $\pi r_s / 2$ (one-fourth of the circumference) and β of the order u_∞ / r_s in Equation (4.4), the gas-phase Nusselt number for both the stagnation point and the flat plate cases was shown to be of the form

$$Nu = - \frac{k f(0) Re^{1/2}}{B'} \quad (4.9)$$

where k was a constant of order unity in both cases. In the stagnation point case, k was slightly larger than in the flat plate case. It was believed that the Nusselt number would decrease monotonically from the stagnation point to the shoulder region and then become negligibly small in the separated region. It was then suggested that the Nusselt number for the whole droplet would be of the same order of magnitude as the Nusselt numbers for the two regions. It was further suggested that a weighted average of the stagnation point Nusselt number and the shoulder region Nusselt number could approximate the droplet Nusselt number. This weighted average approach will be followed in the present study. In particular, the constant A in Equation (4.4) is considered to be given by $A = m(\rho_o \mu_o u_o / r_s)^{1/2}$ where m is a constant which serves as a weighing factor between the stagnation point region and the flat plate region for representing the vaporization rate of the total droplet. The value of m which yields the best agreement with the results of the more exact analysis of Prakash and Sirignano is considered to be the optimum weighing factor.

In Equation (4.5), u_s/u_∞ appears as a parameter in the boundary condition. It was found by Prakash [16] that the surface velocity is typically small and does not greatly affect the heat and mass transfer or the vaporization rate. Because of that the surface velocity can be neglected in the gas-phase analysis. This approximation greatly simplifies the problem by eliminating the matching of the surface velocity along the droplet interface. Although this approximation leads to the physically unrealistic slip condition at the boundary, it is believed that the solution will not be affected significantly.

The boundary conditions in Equation (4.5) become

$$\begin{aligned}
 & \text{(i) at } \eta = 0, \frac{df}{d\eta} = 0 \\
 & \text{(ii) at } \eta = \infty, \frac{df}{d\eta} = 1 \\
 & \text{(iii) at } \eta = 0, \frac{d^2f}{d\eta^2} = \frac{-f}{B'} \quad (4.10)
 \end{aligned}$$

Equations (4.1) and (4.10) form a complete system for the unknown function f . That is, at any time instant, if the surface temperature is known, the B' can be calculated from Equation (4.7) and the function f can be obtained by numerically integrating Equation (4.1) in conjunction with the boundary conditions in Equation (4.10). It should be noted that only the value of f at the interface, i.e., $\eta=0$ is needed for the present study.

Equations (4.1) and (4.10) are similar to the equations in the Emmons' problem [17]. They are indeed almost identical except that the f 's and η 's are differed by a factor of $2^{1/2}$ and $2^{-1/2}$, respectively. Emmons solved the equations numerically for a wide range of values of B' . In the present study, instead of solving Equations (4.1) and (4.10), the results of Emmons' analysis has been utilized. Linear interpolation is used for values of B' which lie between those reported by Emmons.

In Equations (3.15), q_1 is proportional to the liquid-phase heat flux given by Equation (4.8) and thus coupled to the gas-phase solution. At any given time instant, with known surface temperature, the B' can be calculated from

Equation (4.7) and the Blasius function $f(0, B')$ can be obtained using Emmons' results. Subsequently, the liquid-phase heat flux $\lambda_l \partial T / \partial y|_l$ can be evaluated from Equation (4.8). Now the interior droplet temperature distribution can be obtained by solving the heat diffusion equation, Equation (3.10) and its boundary conditions, Equation (3.15). So basically the gas-phase solution and the liquid-phase solution are coupled through the liquid droplet surface temperature. Various solution schemes are used for the coupled vaporization problem. The details are reported in this next chapter.

CHAPTER 5

SOLUTION OF THE COUPLED PROBLEM

5.1. Introduction

The solution to the coupled vaporization problem is given in this chapter. The simplified one-dimensional gas-phase model obtained earlier is coupled to the simplified liquid-phase analysis derived in chapter 3. The resulting coupled formulation for the droplet vaporization can be expressed in the form of a parabolic partial differential equation or a Volterra type integral equation. In the former case the unknown function is the liquid temperature inside the droplet and in the latter case the unknown function is the droplet surface temperature.

The solution of the coupled vaporization problem is first obtained by using a finite difference scheme. The constant m in the coefficient A of the simplified gas-phase solution is optimized to yield the best agreement with the results of the more detailed model of Prakash and Sirignano [2]. The dependence of the optimum value of m on the ambient gas-phase temperature as well as with different fuels is also examined.

An integral formulation which reduces the problem from a multi-dimensional, time dependent formulation to only a time dependent analysis for the droplet surface temperature is obtained. It is found that the integral equation formulation can also be transformed into a system of coupled first order ordinary differential equations. The details of the various formulations and the solution schemes for the coupled vaporization problem are presented in the following sections.

5.2. Finite Difference Solution

In the simplified liquid-phase analysis, the liquid droplet temperature is governed by

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + (1 + C\phi) \frac{\partial T}{\partial \phi} \quad (5.1)$$

where

$$d\tau = \frac{b_1}{b_0} \frac{a_\ell}{R^2} dt \quad (5.2)$$

and

$$C = C(\tau) = 2 \left(\frac{R_0}{R} \right)^{3/2} \frac{d}{d\tau} \left(\frac{R}{R_0} \right)^{3/2} \quad (5.3)$$

In Equation (5.2), t is the physical time; b_0 , b_1 are constants used in the g_1 , g_2 approximations and τ is the non-dimensional time. In Equation (5.3), $C(\tau)$ relates to the droplet vaporization rate and is coupled to the gas-phase solution through the mass vaporization rate.

The initial and boundary conditions are

$$(i) \text{ at } \tau = 0, T = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$$

$$(iii) \text{ at } \phi = 1, \frac{\partial T}{\partial \phi} = q_\ell \quad (5.4)$$

In the simplified gas-phase analysis, the liquid-phase heat flux is given by

$$\lambda_{\ell} \frac{\partial T}{\partial y} \Big|_{\ell_s} = -A f(o) \left[\frac{h_g - h_s}{B'} - L \right] \quad (5.5)$$

The modified Spalding transfer number, B' , is related to the fuel concentration, Y_{fs} , at the droplet surface by

$$B' = \frac{Y_{fs}}{1 - Y_{fs}} \quad (5.6)$$

Here Y_{fs} is a function of the surface temperature given by some equilibrium vapor pressure equation such as the Clausius-Clapeyron equation.

In Equation (5.4), q_{ℓ} is proportional to the liquid-phase heat flux given by Equation (5.5) and is therefore coupled to the gas-phase solution. At any given time instant with known surface temperature, B' can be calculated from Equation (5.6) and the Blasius function $f(o, B')$ can be obtained using Emmons' results. Subsequently, the liquid-phase heat flux $\lambda_{\ell} (\partial T / \partial y)_{\ell_s}$ can be evaluated from Equation (5.5) and the coefficient C can be calculated from the gas-phase solution through Equation (5.3). Next, the interior droplet temperature distribution can be obtained by solving the heat diffusion equation, Equation (5.1), and its boundary conditions, Equations (5.4), via a finite difference method. The new droplet surface temperature is used for the gas-phase solution for the next time step. The same solution scheme is repeated at each time increment and the solution is marched forward in time.

The solutions for hexane and decane vaporizing at various ambient gas-phase temperatures have been obtained by using a Crank-Nicolson type finite difference scheme. The results are shown in Figures 5.1 - 5.8. In these

calculations, the initial droplet temperature is 300°K ; the system pressure is 10 atmospheres and the initial Reynolds number is 100. The physical properties and other conditions are the same as those used in Prakash and Sirignano's study [2]. The droplet surface temperature, the non-dimensional droplet radius and the coefficient C are chosen for comparison with the results obtained from using Prakash and Sirignano's model. For the surface temperature, it was found that [16] the temperature variation along the surface is significant initially, but becomes very small in a time which is short in comparison to the droplet lifetime. This is due to the liquid motion and also due to the fact that the heat flux into the liquid is higher when the surface temperature is lower. Therefore, the surface temperature at the $\theta = 90^{\circ}$ point represents the surface temperature fairly well after a short initial time period. In the present study, the surface temperature of Prakash and Sirignano's model is taken at $\theta = 90^{\circ}$ point for the surface temperature comparison.

The results for hexane and decane at 1000°K gas temperatures are shown in Figures 5.1 through 5.6. The optimum constant m is $(4/\pi)^{1/2}$ for both fuels and the results are in good agreement. The dependence of m on the ambient gas temperature is examined. Results for $T_{\infty} = 700, 1000, \text{ and } 1500^{\circ}\text{K}$ for hexane and $T_{\infty} = 750, 1000, \text{ and } 1200^{\circ}\text{K}$ for decane are obtained. The optimum m remains basically unchanged in all these cases except the hexane case with $T_{\infty} = 1500^{\circ}\text{K}$ where the optimum m is increased slightly to $(4.5/\pi)^{1/2}$. The results shown in Figures 5.1 through 5.6 are all in reasonable agreement with the results of Prakash and Sirignano's model. The percentage disagreement between the two models is reported in Table 5.1. The uncertainty for the optimum value of m is about ± 0.07 for all the cases studied.

The variation of the droplet surface temperature and the vortex center temperature, based on the present simplified model, are shown in Figures 5.7

and 5.8. The vortex center temperature is considerably lower than the droplet surface temperature for a significant portion of the droplet lifetime. The results indicate that the droplet vaporization is essentially unsteady for most of its lifetime, particularly so for the heavier fuel decane at a lower ambient gas temperature. In addition, the droplet heating is unsteady and the droplet temperature becomes uniform only towards the latter part of its lifetime.

As mentioned earlier, the coupled vaporization problem can also be formulated as an integral equation form with the surface temperature being an unknown function of time. The non-vaporizing case is solved in Appendix A. It is important to know that only the droplet surface temperature is needed for determining the vaporization rate and the interior droplet temperature is not needed for determining the heat flux to the droplet and its vaporization rate. The advantage of the integral equation formulation is that it reduces the problem from a multi-dimensional, time-dependent formulation to only a time-dependent analysis for the droplet surface temperature; thereby, eliminating the spatial dependence from the problem.

Table 5-1: Percentage Disagreement Between the Two Models

	HEXANE			DECANE		
Gas Temperature (°K)	700	1000	1500	750	1000	1200
Surface Temperature	N*	2.3%	1.2%	5.0%	2.0%	1.5%
Droplet Radius	N*	N*	N*	N*	1.9%	N*
Coefficient C	5.8%	2.6%	2.9%	11.1%	7.3%	6.8%

*N = Negligible

5.3. Ordinary Differential Equation Solution via Integral Equation Formulation

By using the series solutions of the unity temperature gradient boundary condition case as a Green's function in a Duhamel Integral type superposition scheme, the temperature for the time varying temperature gradient boundary condition case can be obtained. This is basically the procedure for the integral equation formulation.

The cases where $C = 0$, $C = C_0 = \text{constant}$, and $C = -k \tanh(kr/2)$ are considered here. Recall C is the coefficient in the liquid-phase diffusion equation.

For $C = 0$, the temperature inside a droplet, denoted as $K(\tau, \phi)$ here, for the unity temperature gradient boundary condition case, is given by Equation (3.3) as

$$K(\tau, \phi) = \phi - \frac{\phi_0}{2} + \tau - 4\phi_0 \sum_{n=1}^{\infty} \frac{J_0(\lambda_n (\phi/\phi_0)^{1/2})}{\lambda_n^2 J_0(\lambda_n)} \exp(-\lambda_n^2 \tau / 4\phi_0) \quad (5.7)$$

where

$$J_1(\lambda_n) = 0. \quad (5.8)$$

Then by means of the Duhamel's integral technique, the temperature for the time varying temperature gradient boundary condition where $\partial T / \partial \phi = f(\tau)$, is given by

$$T(\tau, \phi) = K(0, \phi) f(\tau) + \int_0^\tau f(x) \frac{\partial K(\tau-x, \phi)}{\partial \tau} dx \quad (5.9)$$

Letting $\phi = \phi_0 = 1$ yields the droplet surface temperature, T_s , which after some rearrangements becomes

$$T_s(\tau) = \int_0^\tau f(x)dx + \sum_{n=1}^{\infty} \left[\int_0^\tau f(x) \exp(-\lambda_n^2(\tau-x)/4) dx \right] \quad (5.10)$$

Which is an integral equation of the Volterra type.

By defining,

$$g_0(\tau) \equiv \int_0^\tau f(x)dx \quad (5.11)$$

and

$$g_n(\tau) \equiv \int_0^\tau f(x) \exp(-\lambda_n^2(\tau-x)/4) dx ; n \geq 1 \quad (5.12)$$

Equation (5.10) can be written as

$$T_s(\tau) = \sum_{n=0}^{\infty} g_n(\tau) \quad (5.13)$$

where at $\tau = 0$.

$$g_n(0) = 0 ; \text{ for all } n \geq 0 \quad (5.14)$$

Taking the τ derivatives of g_i 's gives

$$\frac{dg_0}{d\tau} = f(\tau) \quad (5.15)$$

and

$$\frac{dg_n}{d\tau} = -\frac{\lambda_n^2}{4} g_n(\tau) + f(\tau) ; n \geq 1 \quad (5.16)$$

Now the integral equation formulation of (5.10) is converted completely into a system of first order ordinary differential equations, (5.15) and (5.16),

together with the initial conditions (5.14). The O.D.E. formulation is similar to the approach used in [18] for droplet vaporization with spherical diffusion limit model in the liquid-phase. In that study, the droplet surface regression is neglected in order to obtain a series solution to the heat diffusion equation.

Similarly, for the $C = C_o = \text{constant}$ case, the droplet temperature for the unity temperature gradient boundary condition case where $\partial T / \partial \phi = 1$ is given by Equation (3.27) as

$$K(\tau, \phi) = \frac{\tau + F_s(o, C_o, \phi)}{G_s(o, C_o, \phi_o)} - \frac{1}{2} \frac{G_{ss}(o, C_o, \phi_o)}{G_s^2(o, C_o, \phi_o)} + \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_o, \phi)}{\lambda_n G_s(\lambda_n, C_o, \phi_o)} \exp(\lambda_n \tau) \quad (5.17)$$

where

$$G(\lambda_n, C_o, \phi_o) = 0 \quad (5.18)$$

The temperature for the time varying temperature gradient boundary condition where $\partial T / \partial \phi = f(\tau)$, is as before given by Equation (5.9).

Subsequently, after some mathematical manipulations, the surface temperature is governed by the following integral equation

$$T_s = a \int_0^{\tau} f(x) dx + \sum_{n=1}^{\infty} \left[\beta_n \int_0^{\tau} f(x) e^{\lambda_n(\tau-x)} dx \right] \quad (5.19)$$

where, for brevity,

$$a \equiv \frac{1}{G_s(o, C_o, \phi_o)} \quad (5.20)$$

and

$$\beta_n \equiv \frac{F(\lambda_n, C_0, \phi_0)}{G_s(\lambda_n, C_0, \phi_0)} \quad (5.21)$$

By defining,

$$g_0(\tau) = a \int_0^\tau f(x) dx \quad (5.22)$$

and

$$g_n(\tau) = \beta_n \int_0^\tau f(x) e^{\lambda_n(\tau-x)} dx ; n \geq 1 \quad (5.23)$$

Equations (5.13) and (5.14) become valid. Taking the τ derivatives of g_i 's yields

$$\frac{dg_0}{d\tau} = af(\tau) \quad (5.24)$$

and

$$\frac{dg_n}{d\tau} = \lambda_n g_n(\tau) + \beta_n f(\tau) ; n \geq 1 \quad (5.25)$$

Finally, for the time varying C case where $C = -k \tanh(k\tau/2)$, we have from Equation (3.39)

$$K(\tau, \phi) = \frac{W(0, k, \phi)}{W_\phi(0, k, \phi)} + \sum_{n=1}^{\infty} \frac{W(\lambda_n, k, \phi)}{\lambda_n W_{s\phi}(\lambda_n, k, \phi_0)} \exp(\lambda_n \tau) \quad (5.26)$$

where

$$W_\phi(\lambda_n, k, \phi_0) = 0 \quad (5.27)$$

Recall that a transformation from T to V has been used in this case and $K(\tau, \phi)$ is actually the solution for V with $\partial V / \partial \phi = 1$ at the surface.

The solution for $\partial V / \partial \phi = f(\tau)$ is again given by Equation (5.9) but with T replaced by V . Subsequently, the solution of V at the droplet surface, V_s , can be shown to be given by

$$V_s(\tau) = \sum_{n=1}^{\infty} \left[\gamma_n \int_0^{\tau} f(x) e^{\lambda_n(\tau-x)} dx \right] \quad (5.28)$$

where

$$\gamma_n \equiv \frac{W(\lambda_n, \phi_o, k)}{W_{\phi_s}(\lambda_n, \phi_o, k)} \quad (5.29)$$

By defining

$$g_n(\tau) \equiv \gamma_n \int_0^{\tau} f(x) e^{\lambda_n(\tau-x)} dx ; n \geq 1 \quad (5.30)$$

Equation (5.28) becomes

$$V_s(\tau) = \sum_{n=1}^{\infty} g_n(\tau) \quad (5.31)$$

where at $\tau = 0$,

$$g_n(0) = 0; n \geq 0 \quad (5.32)$$

Again, taking the derivatives of g_i 's with respect to τ gives

$$\frac{dg_n}{d\tau} = \lambda_n g_n(\tau) + \gamma_n f(\tau); n \geq 1 \quad (5.33)$$

Now, the problem has become a system of first order ordinary differential equations.

It should be mentioned that the only additional approximation made in these integral equation formulation is the coefficient C in the liquid-phase diffusion equation. It was pointed out in [12] that during the initial droplet lifetime, transient heating is significant and an accurate solution is essential. Since vaporization is not effective at this stage, the convective term, which is proportional to the surface regression rate represented by C , is negligible. That is, during the active droplet transient heating period, the characteristic internal heat conduction rate is much faster than the surface regression rate such that the location of the droplet surface can be assumed to be frozen during a characteristic thermal wave propagation time. The convective term may become important when significant vaporization proceeds after the active droplet heating. But then an accurate solution of temperature is not essential anymore. It was further pointed out that for a droplet undergoing pure vaporization in a relatively low temperature environment, the droplet regression term probably is always negligible. The effect of the regression term for single-component droplet vaporization will be examined here. In the case of multicomponent droplet, due to large Lewis number, the regression term cannot be neglected in the mass diffusion equation. This will be discussed in the next chapter.

The results of the ordinary differential equation have been obtained for fuel of different volatility vaporizing in a high temperature ambient. A second order Runge-Kutta scheme is used. The results for all three cases are identical to the results of corresponding finite difference solution (i.e. with the same C approximation in the liquid-phase diffusion equation), guaranteeing the accuracy of the ordinary differential equation solutions. These results are also compared with the finite difference solutions with exact C in the equation.

Attempts have been made to extend the solutions of the constant C case to

the varying C case. The solution at any given time is obtained by treating C as constant and computing the O.D.E. solution of the constant C case. However, the "constant" value of C is set equal to the value of C evaluated at the given time. In other words, C is treated as piecewise constant.

The solutions for hexane, decane and hexadecane vaporizing at 1000°K ambient gas temperature have been obtained. The results are shown in Figures 5.9-5.21. The physical properties and other conditions are the same as those used in the last section.

The results of using piecewise constant C are almost identical to the results of using exact C . In fact, the two results are not distinguishable within the accuracy of the plots. In the piecewise constant C scheme, at any given time, the O.D.E. formulation for the constant C case is used with C being treated as constant. The "constant" value of C is updated whenever the difference between the actual value of C and the value of the constant C exceeds a prescribed value, ΔC . Then the new "constant" value of C is set equal to the value of C at the given time. The value of ΔC used in the calculations is 0.05. It was found that with larger value of ΔC , pulses could occur at the discontinuity points where step changes in C occurred.

The results of using $C = \text{constant} = -0.6$ are in closer agreement than the results of using $C = -k \tanh(k\tau/2)$ with $k = 0.8$, which in turn are in closer agreement than the results of using $C = 0$. The timewise variation of C for the three different fuels as well as the various C approximations are shown in Figure 5.21. Since the discrepancies in the results are solely due to differences in approximating C , Figure 5.21 shows that the better C approximation leads to better agreement in results.

The results of using $C = 0$ have the largest disagreement. If reasonably

accurate solutions are needed, the surface regression term should be included in the diffusion equation. As will be shown in the next chapter, due to large Lewis number, the regression term cannot be neglected in the mass diffusion equation since the gradients are larger.

In general, the timewise variation of C is not known a priori. Therefore, it is not obvious which constant C or which constant k should be used in the $C = \text{constant}$ or $C = -k \tanh(k\tau/2)$ approximations. On the other hand, in the piecewise constant C case, the "constant" value of C is known and is equal to the C evaluated at the given time. Therefore, the piecewise constant C approximation, besides having the best agreement, is a more general and useful scheme.

The computational efficiencies of the finite difference solution and the O.D.E. solution have been studied. The results are given in the next chapter.

CHAPTER 6

MULTICOMPONENT FUEL DROPLETS

6.1. Introduction

The recent increase in the utilization of synthetic and derived fuels has resulted in interest in studying the vaporization and combustion of multicomponent liquid fuel droplets (3,5,6,11,25,27,34-39). The fuel vaporization process is crucial in determining the bulk combustion characteristic of a spray combustor. As a fuel droplet travels through a combustor, the more volatile fuel vaporizes earlier while the less-volatile fuel vaporized later. This implies that certain regions will be relatively rich in the more volatile fuel vapors while other regions are relatively rich in the less volatile fuel. This nonuniform distribution of fuel is believed to have considerable influence on the characteristics of ignition, flame stability, and pollutant formation. Therefore, an accurate prediction of composition of the fuel vapor evaporating at the droplet surface is important for spray combustion design analysis.

Law [39] solved the problem of unsteady combustion of a multicomponent fuel droplet in a stagnant, unbounded atmosphere. In that study, the composition and temperature within the droplet were both assumed to be spatially uniform but temporally varying. Sample solutions were obtained and the results indicated that the components vaporize approximately sequentially in the order of their relative volatilities and that the vaporization rate is insensitive to the mixture composition during combustion as well as during pure vaporization in hot environments. It was argued that the model is relevant for less viscous mixtures when internal circulation is so fast that the droplet temperature and compositions are maintained spatially uniform although

temporally varying. Other researchers who share this view refer to the model as rapid mixing model in the literature. As mentioned in Chapter 2, Sirignano [11] showed that even in the limit of high vortex strength, the internal liquid circulation can only reduce the characteristic length scale for diffusion by a factor of three. The rapid mixing limit can never exist. Rather, it would be conceptually more correct to think that the uniform temperature and composition limit results from the infinite diffusivity limit. Therefore it is more appropriate to call it an infinite diffusivity model.

In the absence of internal circulation, only diffusion transport takes place inside the droplet. Since liquid fuels have large Lewis number, the liquid phase mass diffusion rate is very slow compared with that for droplet surface regression and liquid-phase thermal diffusion. Landis and Mills [35] investigated the pure vaporization of a two-component droplet in a stagnant atmosphere. Solutions to equations governing the unsteady mass and heat diffusions within the droplet were obtained by a finite difference method. As in [39], a quasi-steady model of mass and energy transport was used in the gas phase. Results were presented for pentane-, hexane-, and heptane-octane droplets evaporating into air at 1 atmosphere and 600-2300°K. Evaporant composition and vaporization rates were compared with batch distillation behavior and significant differences were noted.

Law [36] generalized the formulation of Landis and Mills to the case of multicomponent droplet which can undergo either pure vaporization or combustion. Results on the vaporization of a binary droplet showed that owing to the significant resistance to diffusion in the liquid phase, the vaporization process approximately consists of an initial transient regime, an intermediate diffusion limited regime which is almost quasi-steady, and a final volatility limited regime. It was further demonstrated that the entrapment of

the volatile components within the rapidly heated interior may lead to the initiation of either homogeneous or heterogeneous nucleation, which can result in the fragmentation of the parent droplet due to the internal pressure buildup. An ideal solution behavior for the mixture was assumed in all these calculations.

As pointed out in [7,39], theoretical analysis for the multicomponent droplet presents several complexities absent in a similar analysis for the single-component droplet. First, the phase-change process at the multicomponent fuel droplet surface and the transport of fuel vapor mixture in the gas phase need to be properly described. Secondly, the numerical efforts are complicated by the stiffness of the coupled governing equations because of the much faster thermal diffusion rate compared with the mass diffusion rate.

The studies discussed thus far are based on the model of spherical symmetry. As mentioned before, the practical problem of droplet vaporization in a spray involves a convective situation in which there is a relative gas-droplet velocity. Empirical correlations such as the Ranz-Marshall type have been applied [27] to the multicomponent droplet to account for the convective effect. Recently, the problem of convective, transient vaporization of multicomponent droplets was analysed by Lara-Urbaneja and Sirignano [3]. Basically, they followed the same arguments used in Prakash and Sirignano's single-component droplet study and extended the analysis to the multicomponent droplet case. The following are the conclusions they made in their study:

1. The transient behavior prevails throughout the history of the droplet for both heat and mass transfer, for the conditions analysed.
2. Even though liquid circulation time is fast, gradients of both temperature and mass prevail at all times, demonstrating the errors of the rapid-mixing concept where uniform composition and temperature are often assumed in this limit.

3. The more volatile component vaporizes early from the surface, yet remains inside the core due to high Schmidt number.
4. The temperature history is controlled by the lighter component initially and then by the heavy component after exceeding the boiling temperature of the lighter component.

In this chapter, similar to the extension of Prakash and Sirignano's analysis by Lara-Urbaneja and Sirignano, the simplified analysis developed for the single-component droplet is extended to the multicomponent droplet case. The details of the extension are given in the next section. As in the single-component droplet case, the resulting coupled formulation for the droplet vaporization can be expressed in the form of a parabolic partial differential equation or a Volterra type integral equation. The integral equation formulation can be transformed into a system of coupled first order ordinary differential equations.

The solution of the coupled vaporization problem is first obtained by using a finite difference scheme. The results of this simplified analysis for a heptane dodecane bicomponent droplet case are compared with the results of infinite-diffusivity limit model and diffusivity-limit model discussed earlier. The details of the formulations of the latter two models can be found in [39] and [35,36] respectively and are not reproduced here.

6.2. Extension of the Single-Component Droplet Analysis and the Finite Difference Solution

6.2.1. Extension of the single-component droplet analysis

Since the simplified analysis for the multicomponent droplet is a direct extension of the simplified analysis of the single-component droplet case previously derived; for the sake of brevity, the complete details of the analysis will not be repeated here. Instead, only the modifications related to the multicomponent droplet extension will be described.

In the gas-phase analysis, the modified Spalding transfer number, B' , is given by

$$B' = \frac{Y_{fgs}}{1 - Y_{fgs}} = \frac{Y_{igs}}{\epsilon_i - Y_{igs}} \quad (6.1)$$

where Y_{fgs} denotes the total fuel vapor mass fraction at the droplet surface and is given by

$$Y_{fgs} = \sum_i Y_{igs} ; \quad i = \text{fuel species} \quad (6.2)$$

ϵ_i is the fractional mass vaporization rates of fuel species i . The subscripts f , g , l and s denote fuel, gas-phase, liquid-phase and droplet surface, respectively. Equation (6.1) is for pure vaporization in an environment free of fuel vapor. It can be shown easily that

$$\epsilon_i = Y_{igs} / Y_{fgs} \quad (6.3)$$

For the interphase conditions, the liquid-phase heat flux at the droplet surface is given by

$$k_{l \frac{\partial T}{\partial y}} \bigg|_{\ell_s} = \rho v (L' - L) \quad (6.4)$$

where L is the latent heat of vaporization and is given by

$$L = \sum_i \epsilon_i L_i; \quad i = \text{fuel species} \quad (6.5)$$

Similarly, the liquid-phase concentration gradient for species i at the droplet surface is given by

$$\left. \frac{\partial Y_{il}}{\partial r} \right|_{rs} = Le \frac{C_{pl}}{k_l} (Y_{ils} - \epsilon_i) \rho v \quad (6.6)$$

For the liquid-phase analysis, the unsteady heat and mass diffusion equations are given respectively by

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + (1 + C\phi) \frac{\partial T}{\partial \phi} \quad (6.7)$$

and

$$\frac{\partial Y_{il}}{\partial \tau} = \frac{\phi}{Le} \frac{\partial^2 Y_{il}}{\partial \phi^2} + \left(\frac{1}{Le} + C\phi \right) \frac{\partial Y_{il}}{\partial \phi} \quad (6.8)$$

where C and τ are as defined in Equations (5.3) and (5.2), respectively. The initial and boundary conditions for the temperature remain the same as in Equation (5.4). For the mass concentration, the initial and boundary conditions are given by

$$(i) \quad \text{at } \tau = 0, Y_{il} = Y_{ilo}$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial Y_{il}}{\partial \phi} = Le \frac{\partial Y_{il}}{\partial \tau}$$

$$(iii) \quad \text{at } \phi = 1, \frac{\partial Y_{il}}{\partial \phi} = f_i \quad (6.9)$$

Here f_i relates to the liquid-phase concentration gradient, $\partial Y_{i\ell} / \partial y|_{\ell}$, as given by Equation (6.6). $Y_{i\ell_0}$ is the initial liquid-phase concentration of species i .

At any given time instant, with known droplet surface temperature, T_s , and liquid-phase species mass fractions, $Y_{i\ell_s}$, at the surface, the gas-phase species mass fractions at the droplet surface, Y_{igs} , can be obtained by means of Raoult's law

$$X_{igs} = X_i^o X_{i\ell_s} \quad (6.10)$$

in conjunction with the Clausius-Clapeyron relation

$$X_i^o = \frac{1}{p_{\infty}} \exp \left\{ \left(\frac{L_i}{R_i} \right) \left(\frac{1}{T_{bi}} - \frac{1}{T_s} \right) \right\} \quad (6.11)$$

X_i^o is the gas-phase mole fraction of species i at the droplet surface when the liquid is pure (i.e. contain species i only). Combining Equations (6.10) and (6.11) yields

$$X_{igs} = \frac{X_{i\ell_s}}{p_{\infty}} \exp \left\{ \left(\frac{L_i}{R_i} \right) \left(\frac{1}{T_{bi}} - \frac{1}{T_s} \right) \right\} \quad (6.12)$$

The mass fractions Y_i 's and the mole fractions X_i 's are related by

$$Y_i = X_i W_i / \sum X_i W_i \quad (6.13)$$

and

$$X_i = Y_i / W_i / \sum (Y_i / W_i) \quad (6.14)$$

where W_i is the molecular weight of species i and i = fuel species plus air for gas; or fuel species only for liquid. Therefore, given T_s and $Y_{i,s}$, $X_{i,s}$ can be obtained from Equation (6.14) which yields $X_{i,g}$ from Equation (6.12) and $Y_{i,g}$ and $Y_{f,g}$ can be determined by Equations (6.13) and (6.12), respectively. Subsequently, B' and ϵ_i can be obtained from Equations (6.1) and (6.3), and the Blasius function can be calculated. The vaporization rate, ρv , can be obtained as in the single-component droplet case. Equations (6.4) and (6.6) then give the liquid-phase heat flux and species mass flux at the droplet surface. The coefficient $C(r)$ can be calculated from the gas phase solution through Equation (5.3). Next, the interior droplet temperature and species concentration distribution can subsequently be obtained by solving the diffusion equations, Equations (6.7) and (6.8) in conjunction with the boundary conditions (5.4) and (6.9) respectively. The new droplet surface temperature and the new liquid-phase mass fractions at the droplet surface are used for the gas-phase solution for the next time step. The same solution scheme is repeated at each time increment and the solution is marched forward in time.

6.2.2. Finite difference solutions

The solutions for heptane-dodecane bi-component droplet vaporizing at various ambient gas-phase temperatures have been obtained for all the three liquid-phase models; namely: the infinite diffusivity model, the spherical diffusion limit model and the vortex diffusion model. Note that the vortex model is basically a diffusion limit model also but with spherical axisymmetry rather than spherical symmetry. In addition, the effects of using different gas-phase models on the vaporization behavior of a bicomponent droplet have also been examined. The gas-phase models include the Ranz-Marshall model and the present simplified model. The vortex model is used in the liquid phase for both cases. The effects of initial liquid mixture composition on

vaporization behavior have also been studied. As in the single-component droplet case, a Crank-Nicolson type finite-difference scheme is used. The results are shown in Figures 6.1 - 6.21. In these calculations, the initial droplet temperature is 300 °K. The ambience is at 1 atmospheric pressure and is free of fuel vapor. The initial droplet diameter is 0.036 cm and the Reynolds number is of the order of 100 throughout the calculations. The physical properties are obtained from [27, 42].

The case which has an ambient temperature of 1000 °K and an initial liquid mass fraction of 50% heptane-dodecane will be used to discuss the salient features of the various liquid-phase models on binary droplet vaporization. The results are shown in Figures 6.1 - 6.6.

Figure 6.1 shows the timewise variations of the surface liquid-phase heptane mass fraction. Significant disagreements exist between the results of the infinite-diffusivity model and the results of the other two models. For both the spherical diffusion limit model and the vortex diffusion limit model, the surface concentration of heptane falls rapidly initially and then levels off at an almost constant value. This is mostly due to the large resistance of mass diffusion within the droplet.

In contrast, for the infinite diffusivity model, the surface mass fraction of heptane decreases steadily with time due to the preferential vaporization of the more volatile species. Eventually, later in the droplet lifetime, the droplet is completely depleted of the heptane component. This result has also been found in [34, 35].

As in the single component droplet case, the results of the vortex model lie in between the results of the other two models. The curves for both the spherical diffusion limit model and the vortex diffusion limit model rise up

slightly later in the droplet lifetime. Initially, the liquid-phase heptane concentration at the droplet surface decreases because the liquid diffusion and convection are too slow to offset the high fractional vaporization rate of heptane. Later on, the fractional vaporization rate of heptane becomes small due to increase in surface temperature and decrease in heptane concentration at the liquid surface. At the same time the liquid convection becomes more important as vaporization becomes more efficient. Eventually, the fast liquid convection and the small fractional vaporization rate of heptane results in a surplus of heptane at the liquid surface.

Figure 6.2 shows the timewise variation of droplet surface temperature. For both the spherical model and the vortex model, the curves rise up rapidly initially and then level off to asymptotically approach the wet bulb temperature. For the infinite diffusivity model, the droplet temperature rises as sensible heat is added, until it approaches the wet bulb temperature. It then continues to increase slowly as the wet bulb temperature increases following the change in the liquid surface composition as shown in Figure 6.1. There is a transition region in between the two inflexion points of the curve which corresponds to the depletion of the heptane component.

Later in the droplet lifetime, the surface temperature of the infinite diffusivity model is considerably higher than the surface temperatures of the other two models even though the heptane compositions at the liquid surface are almost negligible.

Figure 6.3 shows the timewise variation of the overall droplet mass ratio of heptane/dodecane. The results are consistent with those shown in Figures 6.1 and 6.2. Initially, the rapid rise of the droplet surface temperature results in a higher vaporization rate for both the spherical model and the vortex model. Since vaporization is dominated by the more volatile species, the heptane

component near the droplet surface is preferentially vaporized. Hence, initially, the overall droplet mass ratios of the spherical model and the vortex model decrease faster than the infinite-diffusivity model. The latter model predicts a lower surface temperature due to the larger thermal inertia within the droplet.

Afterward, because of large Lewis number, the more volatile heptane component inside the droplet cannot diffuse fast enough to the surface for both the spherical model and the vortex model. This results in a severe limitation for the vaporization of heptane and leads to a large concentration gradient near the droplet surface. Consequently, further decrease in the overall mass ratios of these two models are restricted. In the limit of infinite vaporization rate, each individual vaporization rate will be approximately proportional to its initial concentration and the overall mass fraction of the droplet will remain close to the initial value.

In contrast, for the infinite-diffusivity model, the curve drops steadily with time as a result of the heptane component distilling off more rapidly.

Again the vortex model lies in between the other two models. Distinct differences exist between the three models.

Figure 6.4 shows the timewise variation of the surface gas-phase mass fraction of heptane. The spherical model and the vortex model both predict an initially higher heptane mass fraction as a result of the initial rapid rise in the droplet surface temperature. However, because of the large mass diffusion resistance, a lower value of heptane concentration is subsequently predicted. Later in the droplet lifetime, as the surface temperature slowly rises towards the almost steady wet-bulb temperature, the gas-phase heptane mass fraction increases slightly despite the fact that the liquid-phase heptane mass fraction at the surface remains fairly constant. Note that the wet-bulb temperature

depends upon the species concentration at the droplet surface. Initially the wet-bulb temperature increases as heptane depletes but later on it decreases slowly as the heptane concentration increases gradually.

For the infinite-diffusivity model, the curve rises as the droplet surface temperature increases and subsequently reaches a peak. It then begins to fall to zero as the heptane component inside the droplet is depleted. The increase of the droplet surface temperature and the depletion of the liquid-phase heptane component at the surface have opposite effects on the amount of heptane vapor present at the surface.

Again, as shown on the previous figures, there are considerable disagreements between the infinite diffusivity model and the other two diffusion-limit models.

The timewise variation of the surface fuel vapor mass fraction is shown in Figure 6.5. Initially, the curves for both the spherical model and the vortex model increase rather rapidly. The former model reaches a minor local peak and the latter model levels off locally. This is due to the rapid rise of the surface temperature and the sharp drop of the lighter component concentration beneath the liquid droplet surface, which, according to Raoult's Law, severely limits the vaporization of the lighter component.

For the infinite-diffusivity model, the fuel vapor mass fraction increases initially mainly due to the increase of the droplet surface temperature. Later, as the rate of increase of the droplet surface temperature becomes less and the heptane concentration in the droplet decreases, the fuel vapor mass fraction begins to drop after reaching a peak. Eventually, the fuel vapor mass fraction reaches a minimum and starts to increase again as the droplet reaches complete depletion of the lighter component. Then the droplet surface

temperature begins to rise again at a considerable rate approaching the wet-bulb temperature of the heavier component. Note that the droplet surface temperature closely follows the wet-bulb temperature which depends sensitively on the liquid fuel composition at the surface.

It is interesting that the curve of the vortex model intersects the curve of the spherical model three times. Due to the more rapid increase in the droplet surface temperature, the spherical diffusion limit model has a higher initial vaporization rate. This results in an earlier depletion of the heptane concentration at the liquid surface and a more rapid fall of the overall fuel vapor mass fraction. Subsequently, this leads to the first intersection. Later on as the droplet vaporization resembles more of the heavier component, they intersect again as in the single component case.

Unlike the single component case, the vortex model lies in between the spherical model and the infinite diffusivity model only in the beginning and towards the end of the droplet lifetime. It has been found for the single-component droplet case that the infinite-diffusivity model initially has the lowest fuel vapor mass fraction gradually increases and finally has the highest fuel vapor concentration. The vortex model lies in between throughout the droplet lifetime. In the bicomponent droplet case, as shown in Figure 6.5, there appears to be a large transition region where the above phenomena occurs. This is believed to be caused by the complete depletion of the lighter component predicted by the infinite diffusivity model which results in a drop in the overall fuel vapor mass fraction. The differences between the droplet models are quite significant. As mentioned previously, the distribution of fuel inside a combustor has considerable influence on the combustor characteristics. Therefore, the disagreements in fuel vapor mass fraction predicted by the various models suggest that the overall combustion behaviors will depend on the liquid-phase models used.

The timewise variation of the droplet diameter is shown in Figure 6.6. Again, the vortex model lies in between the other two models only in the beginning and towards the end. This is expected since the vaporization rate closely follows the surface gas-phase fuel mass fraction. The overall differences between the various models are rather insignificant.

In summary, there are substantial differences in the vaporization behaviors between the infinite diffusivity model and the other two models. This is largely due to the neglect of the thermal and mass diffusion resistances.

At short times, the disagreements between the models are caused by the difference in the mode of the thermal energy transfer; while for the bulk of the droplet lifetime, the discrepancies are due to the differences in the mass diffusion models.

The disagreements between the vortex model and the spherical model are relatively less. In fact they both have fairly similar vaporization behaviors. As previously mentioned, due to the large Lewis number, there is a thin boundary layer near the droplet surface for both models. The effects of the boundary layer on the vaporization characteristics are similar for both models. Therefore, the results show a relatively smaller discrepancy than with the infinite-diffusivity model.

The effects of the ambient gas temperature on the bicomponent droplet vaporization behaviors for the various liquid-phase models have been examined. The results for 750 K and 1000 K ambient gas temperature have been obtained. They are shown in Figures 6.7 - 6.12. The results are similar to the previous results of 1000°K ambient gas temperature. There is no significant difference in the disagreements between the different liquid-phase models.

The effects of the gas-phase models on the vaporization behavior of a bicomponent droplet at various ambient gas temperatures are shown in Figures 6.13 - 6.18. The vortex model is used in the liquid phase. The initial liquid-phase mass composition is 50% for all the cases.

There are considerable differences in droplet diameter (Figure 6.18), surface gas-phase fuel mass fraction (Figure 6.17), and surface gas-phase heptane mass fraction (Figure 6.16), between the two gas-phase models. The disagreements in the surface temperature are relatively small except for the high ambient temperature case.

Since the overall mass ratio and the liquid-phase heptane mass fraction depend mostly on the liquid-phase model, the disagreements are rather small.

The disagreements between the two gas-phase models increase as the ambient temperature increases.

The effects of initial liquid-phase mixture composition on the bicomponent vaporization behavior have also been studied. The results from using the present simplified model are shown in Figures 6.19 - 6.21. As was found in [3], although the logical sequence is found; i.e., 50% heptane is always closer in behavior to the pure dodecane case than the 75% heptane case, the curves are not spaced accordingly to their initial composition ratio.

Due to large Lewis number, the liquid-phase mass fraction of dodecane at the droplet surface remains high after the initial rapid drop of the heptane composition. The vaporization behavior of the droplet, except for the initial period, is dominated by the heavier component dodecane.

The larger the initial composition of the heptane component, the larger is the period in which droplet mixture resembles the pure heptane curve. This is consistent with the findings in [3].

6.3. Ordinary differential equation via integral equation formulation

As in the single-component droplet formulation, the cases where $C = 0$, $C = C_0 = \text{constant}$ and $C = -k \tanh(k\tau/2)$ are considered here for the bicomponent droplet. The series solutions for the droplet temperature as well as the ordinary differential equation formulations derived in the previous chapter for the single-component droplet remain valid for the bicomponent droplet.

For the mass diffusion equation, it can be shown that, with a time transformation, the series solutions for the temperature can be extended to yield series solutions for the corresponding mass diffusion equation. Again by using these series solutions as a Green's function in a superposition scheme, solutions for the time varying boundary condition case can be obtained in an integral equation form. Subsequently, by defining some new functions, the integral equation can be transformed into a system of O.D.E.'s. This procedure, which is very similar to the single-component droplet case, is detailed below.

For $C = C_0$ the mass diffusion equation is, from Equation (6.8), given by

$$\frac{\partial Y_{il}}{\partial \tau} = \frac{\phi}{Le} \frac{\partial^2 Y_{il}}{\partial \phi^2} + \left(\frac{1}{Le} + C_0 \phi \right) \frac{\partial Y_{il}}{\partial \phi} \quad (6.15)$$

together with the initial and boundary conditions given by (6.9).

By defining,

$$\tau^* = \tau/Le \quad (6.16)$$

$$Y_{il}^* = Y_{il0} - Y_{il} \quad (6.17)$$

and

$$C_o^* = C_o \cdot Le \quad (6.18)$$

Equations (6.15) and (6.9) become

$$\frac{\partial Y_{il}^*}{\partial \tau^*} = \phi \frac{\partial^2 Y_{il}^*}{\partial \phi^2} + (1 + C_o^* \phi) \frac{\partial Y_{il}^*}{\partial \phi} \quad (6.19)$$

$$(i) \text{ at } \tau^* = 0, Y_{il}^* = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial Y_{il}^*}{\partial \tau^*} = \frac{\partial Y_{il}^*}{\partial \phi}$$

$$(iii) \text{ at } \phi = \phi_o, \frac{\partial Y_{il}^*}{\partial \phi} = -f_i^*(\tau^*) \quad (6.20)$$

where $f_i^*(\tau^*) = f_i(\tau)$

Equations (6.19) and (6.20) resembles Equations (6.17) and (5.4) except for the last boundary condition. The solution, $K(\tau^*, \phi)$, for the unity species gradient boundary condition case where $\partial Y_{il}^* / \partial \phi = 1$ can be obtained from Equation (5.17) by replacing τ and C_o with τ^* and C_o^* respectively. Thus

$$K^*(\tau^*, \phi) = \frac{\tau^* + F_s(o, C_o^*, \phi)}{G_s(o, C_o^*, \phi)} - \frac{1}{2} \frac{G_{ss}(o, C_o^*, \phi_o)}{G_s^2(o, C_o^*, \phi_o)} + \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_o^*, \phi)}{\lambda_n G_s(\lambda_n, C_o^*, \phi_o)} \exp(\lambda_n \tau^*) \quad (6.21)$$

which becomes

$$K(\tau, \phi) = \frac{\tau/Le + F_s(o, C_o^*, \phi)}{G_s(o, C_o^*, \phi_o)} - \frac{1}{2} \frac{G_{ss}(o, C_o^*, \phi_o)}{G_s^2(o, C_o^*, \phi_o)} + \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_o^*, \phi_o)}{\lambda_n G_s(\lambda_n, C_o^*, \phi_o)} \exp(\lambda_n \tau/Le) \quad (6.22)$$

Here the λ_n 's are the roots of

$$G(\lambda_n, C_o^*, \phi_o) = 0 \quad (6.23)$$

Then the solution for the case where $\partial Y_{iL}/\partial \phi = f$ at the surface is, through superposition method, given by

$$Y_{iL}^*(\tau, \phi) = -K(o, \phi)f(\tau) - \int_0^{\tau} f(x) \frac{\partial K(\tau-x, \phi)}{\partial \tau} dx \quad (6.24)$$

Substituting (6.22) into (6.24) gives

$$Y_{iL}^*(\tau, \phi) = -C_1 f(\tau) - \int_0^{\tau} \frac{f(x)}{Le} \left[\frac{1}{G_s(o, C_o^*, \phi_o)} + \sum_{n=1}^{\infty} \frac{F(\lambda_n, C_o^*, \phi_o)}{G_s(\lambda_n, C_o^*, \phi_o)} \exp(\lambda_n (\tau-x)/Le) \right] dx \quad (6.25)$$

where

$$C_1 = \frac{F_s(o, C_o^*, \phi)}{G_s(o, C_o^*, \phi_o)} - \frac{1}{2} \frac{G_{ss}(o, C_o^*, \phi_o)}{G_s^2(o, C_o^*, \phi_o)} \quad (6.26)$$

Setting $\phi = \phi_o = 1$ in (6.25) yields the surface species mass fraction, $Y_{iL}^*(\tau)$, which after some simplifications, becomes

$$Y_{L_s}^*(\tau) = \eta \int_0^\tau f(x) dx + \sum_{n=1}^{\infty} \left[\sigma_n \int_0^\tau f(x) \exp(\lambda_n(\tau-x)/Le) dx \right] \quad (6.27)$$

where

$$\eta = \frac{-1}{Le \bullet G_s(o, C_o^*, 1)} \quad (6.28)$$

and

$$\sigma_n = \frac{-F(\lambda_n; C_o^*, 1)}{Le \bullet G_s(\lambda_n, C_o^*, 1)}; n \geq 1 \quad (6.29)$$

By defining

$$g_o(\tau) \equiv \eta \int_0^\tau f(x) dx \quad (6.30)$$

and

$$g_n(\tau) \equiv \sigma_n \int_0^\tau f(x) \exp(\lambda_n(\tau-x)/Le) dx; n \geq 1 \quad (6.31)$$

Equations (6.27) becomes

$$Y_{L_s}^*(\tau) = \sum_{n=0}^{\infty} g_n(\tau) \quad (6.32)$$

where at $\tau = o$,

$$g_n(o) = o; \text{ for all } n \geq o \quad (6.33)$$

Taking the τ derivatives of g_i 's gives

$$\frac{dg_o}{d\tau} = \eta f(\tau) \quad (6.34)$$

and

$$\frac{dg_n}{d\tau} = \frac{\lambda_n}{Le} g_n(\tau) + \sigma_n f(\tau); n \geq 1 \quad (6.35)$$

Equations (6.33) - (6.35) now form a system of ordinary differential equation which replaces the integral equation (6.27).

For the special case where $C_0 = 0$, we have the series solutions in terms of the Bessel's functions. It can be shown from Equation (5.7) that

$$K(\tau, \phi) = \phi - \frac{\phi_0}{2} + \frac{\tau}{Le} - 4\phi_0 \sum_{n=1}^{\infty} \frac{J_0(\lambda_n (\phi/\phi_0)^{1/2})}{\lambda_n^2 J'_1(\lambda_n)} \quad (6.36)$$

where primes denote derivatives and

$$J_1(\lambda_n) = 0 \quad (6.37)$$

Substituting (6.36) into (6.24) gives

$$\begin{aligned} Y_{\ell}^*(\tau, \phi) = & - \left[\phi - \frac{\phi_0}{2} - 4\phi_0 \sum_{n=1}^{\infty} \frac{J_0(\lambda_n (\phi/\phi_0)^{1/2})}{\lambda_n^2 J_0(\lambda_n)} \right] f(\tau) \\ & - \int_0^{\tau} \frac{f(x)}{Le} \left[1 + \sum_{n=1}^{\infty} \frac{J_0(\lambda_n (\phi/\phi_0)^{1/2})}{J_0(\lambda_n)} \exp(-\lambda_n^2 (\tau-x)/4\phi_0 Le) \right] dx \end{aligned} \quad (6.38)$$

Setting $\phi = \phi_0 = 1$ gives

$$Y_{\ell_s}^*(\tau) = \frac{-1}{Le} \int_0^{\tau} f(x) \left[1 + \sum_{n=1}^{\infty} \exp(-\lambda_n^2 (\tau-x)/4Le) \right] dx \quad (6.39)$$

Defining

$$g_0(\tau) \equiv -\frac{1}{Le} \int_0^\tau f(x) dx \quad (6.40)$$

and

$$g_n(\tau) \equiv -\frac{1}{Le} \int_0^\tau f(x) \exp(-\lambda_n^2(\tau-x)/4Le) dx; \quad n \geq 1 \quad (6.41)$$

we have

$$\frac{dg_0}{d\tau} = -\frac{f(\tau)}{Le} \quad (6.42)$$

$$\frac{dg_n}{d\tau} = -\frac{f(\tau)}{Le} - \frac{\lambda_n^2}{4Le} g_n(\tau); \quad n \geq 1 \quad (6.43)$$

as well as Equations (6.33) and (6.34).

Finally for the time varying C case where $C = -k \tanh(k\tau/2)$, Equation (6.8) becomes

$$\frac{\partial Y_{il}^*}{\partial \tau^*} = \phi \frac{\partial^2 Y_{il}^*}{\partial \phi^2} + (1 + C^* \phi) \frac{\partial Y_{il}^*}{\partial \phi} \quad (6.44)$$

where

$$C^* = C \cdot Le \quad (6.45)$$

It can be shown that

$$C^* = -k^* \tanh(k^* \tau^*/2) \quad (6.46)$$

where

$$k^* = k \cdot Le \quad (6.47)$$

The initial and boundary conditions are given by (6.20).

As was shown in Appendix F, with the following change of variable

$$V^*(\tau^*, \phi) = Y_{i\ell}^*(\tau^*, \phi) \operatorname{sech}\left(\frac{k^* \tau^*}{2}\right) \exp\left(-\frac{k^* \phi}{2} \tanh\left(\frac{k^* \tau^*}{2}\right)\right) \quad (6.48)$$

Equations (6.44) and (6.20) are transformed to

$$\frac{\partial V^*}{\partial \tau^*} = \frac{\partial^2 V^*}{\partial \phi^2} + \frac{\partial V^*}{\partial \phi} - \frac{k^{*2}}{4} \phi V^* \quad (6.49)$$

and

$$(i) \quad \text{at } \tau^* = 0, V^* = 0$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial V^*}{\partial \tau^*} = \frac{\partial V^*}{\partial \phi}$$

$$(iii) \quad \text{at } \phi = \phi_0, \frac{\partial V^*}{\partial \tau^*} = \frac{V^*}{2} \frac{dC^*}{d\tau^*} \quad (6.50)$$

$$= f_{i\ell}^*(\tau^*) \operatorname{sech}\left(\frac{k^* \tau^*}{2}\right) \exp(-C^* \phi_0 / 2)$$

The solution, denoted by $K^*(\tau^*, \phi)$ here, for V^* with $\partial V^* / \partial \phi = 1$ at the droplet surface, can be obtained from Equation (3.39) by replacing k, τ and C with k^*, τ^* and C^* respectively. Hence

$$K^*(\tau^*, \phi) = \frac{W(0, k^*, \phi)}{W_{\phi}(0, k^*, \phi_0)} + \sum_{n=1}^{\infty} \frac{W(\lambda_n, k^*, \phi) e^{\lambda_n \tau^*}}{\lambda_n W_{\phi_s}(\lambda_n, k^*, \phi_0)} \quad (6.51)$$

Here λ_n 's are the roots of

$$W_{\phi}(\lambda_n, k^*, \phi_0) = 0 \quad (6.52)$$

The solution for the case where $\partial V^*/\partial \phi = f^*(\tau^*)$ at the droplet surface is given by

$$V^*(\tau^*, \phi) = K^*(0, \phi) f^*(\tau^*) + \int_0^{\tau^*} f^*(x) \frac{\partial K^*(\tau^* - x, \phi)}{\partial \tau^*} dx \quad (6.53)$$

Substituting (6.51) into (6.53) and setting $\phi = \phi_0 = 1$ yields

$$V_s^*(\tau^*) = \sum_{n=1}^{\infty} \epsilon_n \int_0^{\tau^*} f^*(x) e^{\lambda_n(\tau^* - x)} dx \quad (6.54)$$

where

$$\epsilon_n = \frac{W(\lambda_n, k^*, 1)}{W_{\phi_s}(\lambda_n, k^*, 1)} ; n \geq 1 \quad (6.55)$$

and subscript s in V_s^* denotes droplet surface.

Replacing τ^* by τ , Equation (6.54) becomes

$$V_s(\tau) = \sum_{n=1}^{\infty} \frac{\epsilon_n}{Le} \int_0^{\tau} f(x) \exp\left(\frac{\lambda_n}{Le}(\tau - x)\right) dx \quad (6.56)$$

Note here that

$$V_s^*(\tau^*) \equiv V_s(\tau) \quad (6.57)$$

and

$$f^*(\tau^*) = f(\tau) \quad (6.58)$$

From (iii) or (6.50)

$$f^*(\tau^*) = \frac{V_s^*(\tau^*)}{2} \frac{dC^*}{d\tau^*} - f_i^*(\tau^*) \operatorname{sech}\left(\frac{k^*\tau^*}{2}\right) \exp(-k^*/2) \quad (6.59)$$

Therefore

$$f(\tau) = \frac{V(\tau)}{2Le} \frac{dC}{d\tau} - f_i(\tau) \operatorname{sech}\left(\frac{k\tau}{2}\right) \exp(-k/2) \quad (6.60)$$

Defining

$$g_n(\tau) \equiv \frac{\epsilon_n}{Le} \int_0^\tau f(x) \exp(\lambda_n/Le(\tau-x)) dx; \quad n \geq 1 \quad (6.61)$$

Equation (6.56) becomes

$$V_s(\tau) = \sum_{n=1}^{\infty} g_n(\tau) \quad (6.62)$$

where at $\tau = 0$,

$$g_n(0) = 0; \quad n \geq 1 \quad (6.63)$$

Furthermore

$$\frac{dg_n}{d\tau} = \frac{\epsilon_n}{Le} f(\tau) + \frac{\lambda_n}{Le} g_n(\tau); n \geq 1 \quad (6.64)$$

Finally, from (6.48)

$$Y_{is}^*(\tau) = V_s(\tau) \cosh\left(\frac{k\tau}{2}\right) \exp(C^*/2) \quad (6.65)$$

The results for hexane-dodecane bicomponent droplet vaporizing at 1000°K ambient temperature have been obtained. In these calculations, the initial droplet temperature is 300°K; the system pressure is 10 atmospheres and the initial Reynolds number is 100. The physical properties and other conditions are the same as those used in [2,3]. Although the value of 30 is more representative of typical liquid fuels, Lewis numbers of 1, 10 and 30 are used.

The same C approximations as in the single-component droplet case are examined here. The results are shown in Figures 6.23-6.43.

For all three Lewis numbers, the results of the O.D.E. solutions using $C = 0$ are identical to the results of the corresponding finite difference solutions (i.e. with $C = 0$ in the liquid-phase mass and heat diffusion equations) the accuracy of the O.D.E. solution for the bicomponent droplet case is again confirmed. It has been found that as Lewis number increases, the system becomes stiffer and more equations are needed in the O.D.E. solution.

As in the single component droplet case, with unity Lewis number, the results of the O.D.E. solutions for $C = \text{constant}$, $C = -k \tanh(k\tau/2)$ and $C = \text{piecewise constant}$ agree well with the results of the corresponding finite difference solution (i.e. with the same C approximation in the liquid-phase diffusion equations).

For larger Lewis number, more eigenvalues and equations are needed in the O.D.E. solution. The series solutions generated in Appendices E and G

converge very slowly for large eigenvalues and asymptotic series are needed. Although there are no foreseeable difficulties in obtaining the asymptotic series for the large Lewis number case, the results for $Le = 10$ and 30 are obtained by using the finite difference method. The objective here is to examine the various C approximations.

Later when investigating the computational efficiency of the O.D.E. solution and the finite difference solution schemes, the $C = 0$ case is used. Note that the number of equations in the O.D.E. solution depends mainly on the stiffness of the problem (given by the Lewis number) but not on C , the surface regression rate parameter. In other words, for a given Lewis number, one should expect to use the same number of equations for the various C approximation schemes for the same accuracy.

As in the single-component droplet case, the results of using piecewise constant C are almost identical to the results of using exact C . In some cases, the two results are not distinguishable within the accuracy of the plots. The values of ΔC is 0.05 for unity Lewis number and 0.01 for higher values of Lewis number.

The results of using $C = \text{constant} = -0.6$ are in closer agreement than the results of using $C = -k \tanh(k\tau/2)$ with $k = 0.8$, which in turn are in closer agreement than the results of using $C = 0$. The timewise variation of C for the three different Lewis number cases as well as the $C = -k \tanh(k\tau/2)$ case are shown in Figure 6.43.

The results of using $C = 0$ have the largest disagreement. The results suggest that the surface regression term cannot be neglected in the diffusion equation particularly for the high Lewis number case.

Once again, the piecewise constant C scheme yields the best agreement and is a more general and useful scheme.

The computational efficiencies of the finite difference solution and the O.D.E. solution have been studied. The case $C = 0$ and Lewis number = 30 is considered. Figure 6.44 shows the maximum percentage error in overall mass vaporization rate versus CPU time comparisons. The O.D.E. solution curve appears to lie below the finite difference solution curve which suggests that the former solution scheme is more efficient.

As previously mentioned, only the droplet surface temperature and the liquid surface species concentration are needed for determining the vaporization rate. The interior droplet temperature and species concentration are not needed for determining the heat and mass fluxes to the droplet and its vaporization rate. The advantage of the O.D.E. formulation is that it eliminates the spatial dependence from the problem and results in reduction of computation time.

CHAPTER 7

ONE DIMENSIONAL SPRAY VAPORIZATION STUDY

7.1. Introduction

As mentioned in the introduction section, the main objective of this thesis is to develop an algorithm for the droplet vaporization which is simple enough to be feasibly incorporated into a complete spray combustion analysis and yet will also account for the important physics such as liquid-phase internal circulation, unsteady droplet heating and axisymmetric gas-phase convection. In this chapter, the use of the present simplified model in a spray situation is examined. In particular, a transient one-dimensional flow of an air-fuel droplet mixture in an open tube is considered. The objective is to verify the feasibility of incorporating the present simplified model into a one-dimensional spray vaporization calculation and to demonstrate the potential usefulness of the model in an overall spray calculation.

The physical situation, the mathematical formulation of the problem and its solution procedure are presented in the following sections. The results are discussed in the next chapter.

7.2. Physical Situation and Mathematical Formulation

The physical situation consists of a continuous laminar flow of hot air in an open tube. The gas-phase properties initially in the tube and later at the tube entrance are prescribed. The injection of fuel droplets is intermittent. One group of droplets is injected every given time interval. The number of droplets in a group (or with a characteristic) represents the number of droplets per unit cross-section area. The frequency of injection and initial droplet

velocity depends on the overall fuel-air ratio in the tube, the mass flow of air, droplet spacing and droplet diameter at the tube entrance. The prescription of the overall fuel-air ratio, the droplet diameter and the droplet velocity at the entrance yields the value of the droplet number density. The droplet spacing in the axial direction and the number of droplets per unit cross-section area are adjusted to provide initially an isotropic droplet spacing in a unit cube. Initially a high relative velocity is provided between the two phases. As a droplet group moves in the hot gas stream, it accelerates. At the same time, droplet heating and vaporization are taking place. The spray processes influence the state of the gas, i.e., the gas-phase is continuously retarded, cooled, and enriched with fuel vapor. The gas-phase properties are also being influenced by the upstream convection. All these gas-phase and liquid-phase processes are modeled by a system of unsteady, one-dimensional equations. The gas-phase is represented in Eulerian coordinates whereas the liquid phase is represented in Lagrangian coordinates. The governing equations in the non-dimensional form are given as follows:

In the gas phase,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho V) = S_\rho \quad (7.1)$$

$$\frac{\partial Y}{\partial t} + V \frac{\partial Y}{\partial x} - t_r D \frac{\partial^2 Y}{\partial x^2} = S_Y \quad (7.2)$$

$$Y = Y_f, Y_o, \phi \quad (7.3)$$

$$Y_N = 1.0 - Y_f - Y_o \quad (7.4)$$

$$\phi = TP^{(1-\gamma)/\gamma} \quad (7.5)$$

$$\rho = \frac{p^{(1/\gamma)}}{\phi} \quad (7.6)$$

In the liquid phase,

$$\frac{dX_k}{dt} = V_k \quad (7.7)$$

$$\frac{dV_k}{dt} = \left\{ \rho_r L_r^2 t_r \right\} \left\{ \frac{3}{16} \frac{C_D \mu Re_k (V - V_k)}{S_k} \right\} \quad (7.8)$$

$$\frac{dS_k}{dt} = -2 \left\{ \rho_r L_r^2 t_r \right\} (1 + 0.3 Re_k^{0.5}) \ln(1 + B_k) \quad (7.9)$$

for Ranz-Marshall correlation model

$$\frac{dS_k}{dt} = -2 \left\{ \rho_r L_r^2 t_r \right\} \left[\frac{2}{\pi} Re_k \right]^{0.5} f(B_k) \quad (7.10)$$

for the present simplified model

$$S_k = r_k^2 \quad (7.11)$$

$$C_D = \frac{24}{Re_k} (1 + Re_k)^{2/3} / 6 \quad (7.12)$$

$$Re_k = \frac{2}{t_r L_r} \frac{r_k \rho}{\mu} |V - V_k| \quad (7.13)$$

$$\mu = \mu(T'_{ref}) = \frac{1}{\mu_o} \left[\frac{b_1 T'^{3/2}_{ref}}{b_2 + T'_{ref}} \right] \quad (7.14)$$

$$\text{where } T'_{ref} = \frac{1}{3} T' + \frac{2}{3} T'_k \quad (7.15)$$

The symbols used in the equations above are explained below as well as in Table 8.1. The primes denote dimensional quantities.

The source terms in the gas-phase equations result from the coupling between the two phases. These are given in Appendix B. It should be noted that a transformation as given by Equation (7.5) has been employed. This transformation is useful for a constant volume situation [18]. However, it has been retained here (a constant pressure case) for the sake of generality.

In non-dimensionalizing the gas-phase equations, the length scale is the length of the tube, and the velocity scale is the gas velocity at the tube entrance. The time scale is determined by these two scales. The gas-phase properties are non-dimensionalized by using the respective properties at the entrance. For the liquid-phase equations, the droplet location, velocity and surface temperature are respectively non-dimensionalized by the gas-phase length, velocity and temperature scales. The droplet radius is non-dimensionalized by the initial droplet radius. The above non-dimensionalization gives rise to three additional dimensionless groups, t_r , L_r and ρ_r ; t_r is the ratio of convective time to diffusion time in the gas-phase, L_r is the ratio of gas-phase length scale and initial drop radius, and ρ_r is the ratio of initial gas-phase density and liquid density.

The important assumptions made in these equations are that the gas pressure

is constant, radiative heat transfer is negligible, the species diffusion follows Fick's law with equal mass diffusivities, the specific heat at constant pressure is constant, and the gas-phase Lewis and Schmidt numbers are unity. In addition, the product $\rho D (= \mu)$ is assumed constant. It is noteworthy, however, that in the calculation of liquid-phase properties μ is considered a function of temperature as given by Sutherland correlation [19]. As indicated in Equation (7.14), a reference temperature is used for the calculation of μ and the reference temperature is obtained by 1/3 rule as recommended by Sparrow and Gregg [20].

The drag coefficient is evaluated by using an expression as proposed by Putnam [21]. The evaluation of Reynolds number for the drag coefficient is based on the free stream density and viscosity evaluated at the 1/3 reference state. This follows the recommendation of Yuen and Chen [22]. It should also be noted that the effect of relative droplet-gas velocity on the vaporization rate [see Equations (7.9) and (7.10)] has been treated by a semi-empirical correlation as well as by an axisymmetric model.

7.3. Solution Procedure

A hybrid Eulerian Lagrangian numerical scheme is used to calculate the gas-phase and liquid-phase properties at the $(n+1)^{\text{th}}$ time level from the values known at the n^{th} time level. First of all, a second-order accurate scheme is employed to interpolate the gas-phase properties from the Eulerian locations (fixed grid points) to the Lagrangian (or droplet) locations. The scheme uses the gas-phase properties at two grid points x_i and x_{i+1} and gives the corresponding properties at a Lagrangian location X_k , where X_k is between x_i and x_{i+1} . Using these gas-phase properties, the droplet surface temperature is then calculated. For the infinite conductivity model, it involves the solution of an ordinary differential equation for each droplet group. For the conduction

limit and vortex models, a partial differential equation needs to be solved. The details have been discussed in the previous chapters. Knowing T_k for each droplet group, other droplet properties (X_k , V_k , r_k) can be obtained by solving Equations (7.7) - (7.11). A second-order Runge-Kutta scheme is used for this purpose. It should be noted, however, that there is some loss of accuracy due to the fact that the gas-phase properties are not updated in the Runge-Kutta scheme. Using the new liquid-phase properties, the source terms as given in the Appendix B can be evaluated at the Lagrangian locations. Then a second-order accurate scheme is used to distribute these source terms from a Lagrangian location to the two neighboring gas-phase locations. Using these source terms, the gas-phase properties (Y_i , Y_o and ρ) at the $(n+1)^{th}$ time level are obtained by solving Equation (4.2). An explicit finite-difference method is used for this purpose. The gas temperature and gas density are then obtained by using Equations (4.5) and (4.6). Finally the gas velocity is obtained from an integral form of the continuity Equation (4.1). It is worth emphasizing that in the present case, the gas-phase convection term dominates the diffusion term. Therefore, an upwind difference scheme [15] is employed for the convection term. It should also be noted that an explicit method was found to be the most efficient for reacting two-phase flow [15]. However, an implicit method may be more efficient for the present vaporizing case without combustion since the equations may not be as stiff.

The results have been obtained and are presented in the next chapter where the effects of using different gas and liquid phase models on the bulk spray and gas phase properties are studied.

CHAPTER 8

COMPARISON OF VAPORIZATION MODELS

8.1. Introduction

The effects of different gas and liquid phase models on the vaporization behavior of a single component isolated droplet are studied for both the stagnant and the convection situations. The different liquid-phase models include d^2 -law, infinite conductivity limit, diffusion limit and the present simplified vortex model. The different gas-phase models include a spherically symmetric model in the stagnant case and Ranz-Marshall correlation plus the present simplified axisymmetric gas-phase model. In addition, the detailed model of Prakash and Sirignano [2] is also included.

Liquid fuel droplets initially at 300 K vaporizing in 1000 K, 10 atmospheric pressure fuel-free environment is used to study the various gas-phase and liquid-phase models. Hexane, decane and hexadecane droplets of initial radius .00476 cm are considered. The physical properties are the same as those in the Prakash and Sirignano's analysis [2].

The use of some of these models in a spray situation is also examined. The one-dimensional spray vaporization problem described in the last chapter is used. A critical comparison of all of these models is made.

It is shown that the fuel vapor mass fraction can be very sensitive to the particular liquid-phase and gas-phase models. The results are presented in the following sections.

8.2. Spherically Symmetric Models

The results for the stagnant case are given in Figures 8.1 and 8.2. The gas-phase model is quasi-steady and spherically symmetric. Three different liquid-phase models namely the d^2 -law, the conduction limit and the infinite conductivity limit are compared. Since the existence of a vortex in a stagnant environment cannot be realized conceptually, it is excluded for comparison. One would think that if the vortex model were included, it would be in between the infinite conductivity limit and the conduction limit. This indeed can be shown to be true. Figures 8.1 and 8.2 show the temporal variation in the surface temperature and surface area respectively. The physical time, t is nondimensionalized by using the liquid thermal diffusivity, α_l , and the initial droplet radius, r_0 , as $\tau = t/(r_0^2/\alpha_l)$. For the d^2 -law model the surface temperature is at the wet-bulb temperature and remains constant while the surface area regresses linearly in time. The d^2 -law serves as an asymptotic limit for the other two models. This is reflected in Figure 8.1 where the surface temperature of the other two models approaches the wet bulb temperature and Figure 8.2 where the curves become more linear.

Since the d^2 -law neglects the initial transient droplet heating, the droplet vaporizes much faster than the other two models. The difference is bigger for the heavier fuels which have higher boiling temperatures and hence longer transient heating period. Conversely, the conduction limit and the infinite conductivity limit have about the same droplet lifetime. Note that these two limits intersect each other. Since the droplet temperature is uniform in the infinite conductivity limit, the surface temperature increase per unit of energy absorption is less. Consequently, the fuel vapor mass fraction at the droplet surface is lower, which leads to lower vaporization rate. On the other hand, the difference between the ambient temperature and the surface temperature,

which relates directly to the heat transfer rate to the liquid, is higher. This results eventually in a higher surface temperature and faster vaporization rate during the latter portion of the lifetime for the infinite conductivity model. Note that the wet-bulb temperatures in these calculations are considerably lower than their corresponding boiling temperatures of the fuels. The effect of the different liquid-phase models on the interior liquid temperature is quite significant and therefore the conduction limit model, which is considered to be exact, should be used, if detailed temperature distribution inside the droplet is needed. The infinite conductivity model may be useful in the low ambient temperature case when the droplet lifetime is long. The d^2 -law model which gives poor agreement with the conduction limit model is oversimplified and should be discarded.

8.3. Droplet Vaporization With Convective Effects

The results for the convective case are given in Figures 8.3 to 8.6. In these calculations, the Reynolds number (based on droplet diameter) is initially 200 and decreases with the diameter as the droplet vaporizes. The relative velocity is 2500 cm/sec and is assumed to be constant throughout. In reality the relative velocity will be reduced by the drag force; this is considered later in the spray vaporization case.

Although Prakash and Sirignano's model is the most detailed and should be considered to be the most exact, it is quite cumbersome to be included in a complete spray analysis. Instead, the simplified gas-phase and liquid-phase models of the present study which have been demonstrated in Chapter 5 to give close agreement with Prakash and Sirignano's results are used as reference models in the figures.

Figures 8.3 and 8.4 show the results of the various liquid-phase models. The

d^2 -law does not exist in this convective case. Again, the conduction limit and the infinite conductivity limit intersect due to the same reasoning as that in the stagnant case. The vortex model lies in between the other two models as expected. Note that the droplet lifetime is considerably shorter than that in the stagnant case. In the convective case, $(r/r_o)^{3/2}$ regresses asymptotically linearly with time and it is used in Figures 8.4 and 8.6. Figure 8.4 shows that for the heavier fuel the percentage variation in droplet lifetime can depend quite significantly on the liquid-phase model.

Figures 8.5 and 8.6 show the effects of the different gas-phase models. The Ranz-Marshall correlation overpredicts the vaporization rate and underestimates (for decane) the surface temperature. As indicated by Sirignano [11], this type of correlation has very little theoretical justification and cannot give satisfactory results. The present study supports Sirignano's qualitative analysis. As expected, the simplified one-dimensional model of the present study appears to be in good agreement with the more detailed model of Prakash and Sirignano.

The simplified vortex model applies to a situation where: (a) the streamfunction patterns are described reasonably well by a Hill's spherical vortex pattern and (b) the circulation time is very short compared to other characteristic times. The Hill's spherical vortex can be obtained when the nonlinear inertial terms in the momentum equation can be neglected compared to other terms. This can occur at low Reynolds number via an order of magnitude argument. Fortuitously, in similar fashion to Couette flow or Poiseuille flow, the inertial terms go identically to zero so that the streamfunctions are valid even at higher Reynolds number. The very short circulation time or very high vortex strength implies a very high Peclet number for the liquid (upon comparison of diffusion time to circulation time). Since

Prandtl number is of order ten, a high Reynolds number is implied. For low Reynolds number, the heat conduction will occur in a two-dimensional fashion, both normal and tangent to the streamsurfaces. This complicates the application of a simplified model to a low Reynolds situation. The gas-phase models are also limited to high Reynolds numbers since thin boundary layers are considered. So for several reasons, additional modelling is required if the low Reynolds number case is to be considered.

The results indicate that the droplet heating and vaporization are essentially unsteady for most of its lifetime, particularly for the heavier fuel. For a detailed analysis, Prakash and Sirignano's model is recommended but for more practical application, the simplified model of the present study would be useful.

8.4. One Dimensional Spray Vaporization

The effects of using different liquid-phase models on the bulk spray and gas-phase properties are now discussed. The various values used in the computation are listed in Table 8.1. The criterion used in selecting these values was to consider a spray vaporization situation with a moderate gas-phase convection for the droplets. The selected values provide an initial Reynold's number (based on the relative velocity and the drop diameter) of 113 and a droplet residence time of about 12.5 msec. During this time, eighty percent of the droplet mass is vaporized. The effects of different liquid-phase models on the bulk gas-phase properties is presented in Figures 8.7 - 8.10. Figures 8.7 and 8.8 indicate that the choice of a particular droplet heating model can significantly influence the fuel vapor distribution in the tube. This can have a profound effect on the subsequent combustion process in a practical situation. The maximum difference between the fuel vapor mass fraction values is as much as one hundred percent between the conduction

limit and the infinite conductivity models. As Figure 8.8 indicates, the conduction limit model initially (up to a distance of 5 cm) predicts the highest fuel vapor mass fraction, whereas the infinite conductivity model predicts the lowest. At later times the situation is reversed. The results of present simplified vortex model are always in between those of the other two models. The difference in the fuel vapor distribution is a direct consequence of the difference in the droplet surface temperature values for the three models. As discussed earlier, the conduction limit model initially predicts the highest droplet surface temperature and therefore the fastest vaporization rate, whereas the infinite conductivity model predicts the lowest surface temperature and the slowest vaporization rate. This behavior is reversed at later times.

The fuel vapor mass fraction profiles in Figures 8.7 and 8.8 exhibit an oscillatory behavior. This is due to the periodic nature of the droplet injection process which causes a finite droplet spacing in the streamwise direction. Thus the period of this oscillation is the same as the time interval between two subsequent injections. This is clearly illustrated in Figure 8.9. As this figure indicates the profiles overlap after every 0.5 msec, which is the time interval between two subsequent injections. This unsteady gas-phase behavior, which is entirely due to the spray discretization, should be kept in mind in spray modeling. The gas temperature profiles at time = 16 msec for the three liquid models are shown in Figure 8.10. The continuous drop in the gas temperature is indicative of the continuous cooling of the gas-phase due to droplet heating and vaporization. The difference in the gas temperature distribution due to the different liquid-phase models is not as significant as that in the fuel vapor distribution. This is due to the fact that the spray heating and vaporization constitute only a small heat loss in the overall gas-phase heat budget. The oscillatory behavior in the gas temperature profiles is

again due to the intermittent droplet injection process. This intermittency is prescribed exactly in our idealized calculation. In a practical situation, it may not be so well-defined and perhaps should be taken as random. That is, the distance between droplets as they flow into the domain of interest will not be fixed as they are given in this calculation but rather will be distributed about some average value.

The effect of different liquid heating models on the droplet properties is illustrated in Table 8.2. The properties of the first droplet group, i.e. the location, the non-dimensional radius, the surface temperature, and the velocity are given as functions of time for the three models. The difference in the surface temperature and the droplet radius for the three models is very similar to that discussed previously. The conduction limit model predicts the highest droplet velocity, whereas the infinite conductivity model predicts the lowest value. This occurs since the conduction limit model initially predicts the fastest vaporization rate, the smallest drop size, and consequently the highest droplet acceleration. It should be noted, however, that the difference in the droplet velocities for the three models is quite small.

The effect of different convective models is presented in Figures 8.11 - 8.12. It should be noted that the simplified axisymmetric mode of the present study is valid only when the Reynolds number is large compared to unity; as indicated by Equation (7.10), this model predicts a vaporization rate, which is proportional to the square root of the Reynolds number. For this reason, initial droplet radius of 100 microns is used for these calculations. This gives a value of 226 for the initial Reynolds number. Figure 8.11 shows that the Ranz-Marshall correlation overpredicts the vaporization rate as compared to that given by the axisymmetric model. This behavior is consistent with the one observed for the single droplet case in the previous section. Figure 8.12

gives the differences in the gas temperature distribution for the two models. Since the Ranz-Marshall correlation predicts a higher vaporization rate and therefore a higher heat loss from the gas phase, it gives lower gas temperatures than those given by the correlation.

8.5. Summary

The most common vaporization models have been compared for fuels of varying volatility in a high-temperature environment. Both isolated droplet and spray vaporization have been studied. The use of the d^2 -law or the infinite-conductivity model (sometimes named the rapid mixing model) has been shown to be very inadequate. For spherically-symmetric vaporization (no relative gas-droplet motion), the conduction limit model for transient heating is recommended. In practical situations where a relative gas-droplet motion exists, the simplified vortex model of the present study is recommended when the Reynolds number based on relative velocity is high. That model compares well with the more detailed model of Prakash and Sirignano and predicts well the effects of the laminar gas-phase boundary layer over the droplet and the internal circulation in the droplet.

The spray calculations indicate an inherent unsteadiness due to the intermittent character of a spray. This unsteadiness will be interesting whenever we wish to resolve structure on the scale of the average distance between droplets.

**Table 8-1: Values of Various Parameters
Used in Spray Calculations**

Parameter	Value
Fuel	N-Decane
Liquid Density	$\rho'_k = 0.773$
Initial Drop Radius	$r'_o = 50$ microns
Initial Drop Temperature	$T'_k = 300^\circ\text{K}$
Number of Drops per unit cross-section area	$N'_k = 400 \text{ 1/cm}^2$
Drop spacing in the axial direction	$d'_s = 0.05 \text{ cm}$
Gas velocity at the tube entrance	$V'_c = 1000 \text{ cm/sec}$
Drop Velocity at the tube entrance	$V'_k = 0.1 V'_c$
Tube length	$L_c = 10 \text{ cm}$
Pressure	$p'_c = 10 \text{ atm}$
Gas temperature at the entrance	$T'_c = 1000^\circ\text{K}$
Temporal step size	$\Delta t' = 10^{-5} \text{ sec}$
Spatial step size	$\Delta x' = 0.1 \text{ cm}$
Specific heat at constant pressure	$C'_p = 0.25 \text{ cal/gm}^\circ\text{K}$
Molecular weight of fuel	$M'_f = 142.3 \text{ gm/mole}$
Molecular weight of oxidizer	$M'_o = 32.0$
Boiling temperature of the Fuel at 1 atm	$T'_{bn} = 447.3^\circ\text{K}$
Heat of vaporization	$L' = 86.5 \text{ cal/gm}$
Gas constant	$R'_{\text{gas}} = 2.8393 \text{ atm cm}^3/\text{gm}^\circ\text{K}$

Table 8-2: Properties of the First Droplet Group
for Different Liquid Phase Models

Conduction Limit Model

t(msec)	X_k' (cm)	r_k/r_o	T_k' (°K)	V_k' (cm/sec)
0	0	1.0	300.0	100.0
2	0.885	0.961	445.0	590.0
4	2.272	0.902	453.3	773.1
6	3.916	0.842	458.1	861.2
8	5.691	0.781	462.2	909.2
10	7.540	0.716	465.9	937.2
12	9.433	0.648	469.1	954.5

Infinite Conductivity Model

t(msec)	X_k' (cm)	r_k/r_o	T_k' (°K)	V_k' (cm/sec)
0	0	1.0	300.0	100.0
2	0.889	0.994	412.5	587.6
4	2.257	0.948	459.4	758.2
6	3.869	0.867	471.8	845.0
8	5.615	0.779	474.5	897.1
10	7.445	0.692	475.0	930.3
12	9.328	0.604	475.1	951.6

Vortex Model

t(msec)	X_k' (cm)	r_k/r_o	T_k' (°K)	V_k' (cm/sec)
0	0	1.0	300.0	100.0
2	0.885	0.973	438.1	588.0
4	2.264	0.92	452.6	767.5
6	3.895	0.858	460.6	854.7
8	5.658	0.791	465.6	903.4
10	7.496	0.721	468.8	932.7
12	9.382	0.648	470.9	951.3

CHAPTER 9

COMPARISON WITH EXPERIMENTAL DATA

9.1. Available Experimental Data

There has been considerable experimental work on the problem of single droplet vaporization and combustion, [4,8,9,23-30]. Largely due to experimental difficulties, most of the earlier (prior to [27,28]) experimental studies have employed simplifications which are far removed from reality and hence may have resulted in discrepancies with actual droplet vaporization behavior. These simplifications include:

1. **Suspended droplet:** a single droplet suspended at the end of a thin quartz fiber. The suspending element distorts the shape of the droplet and conducts heat from the hot ambient gas to the droplet interior. The filament also interrupts the internal liquid circulation that may occur in a convective situation. Furthermore, the minimum droplet size is limited by the thickness of the suspension filament which is much larger than typical droplet size inside a spray combustor.
2. **Porous sphere:** a porous sphere with liquid fuel continuously supplied to the droplet interior at a rate that combustion or vaporization at the surface is maintained at a steady state. The main drawback is that transient behavior of the droplet cannot be simulated by the porous sphere.
3. **Stagnant ambient gas phase:** relative gas-droplet velocity neglected. In reality, the practical problem of droplet vaporization in a combustor involves a convective situation in which there is a relative gas-droplet velocity. This relative velocity can significantly increase the vaporization and heat transfer rates. It can also lead to internal liquid circulation through the shear force generated at interface. Also, in most of these earlier experimental studies, the droplet sizes are generally too large and the vaporization rates are too low for a spray combustor. Since the present theoretical model accounts for liquid internal circulation and convective heat and mass transfer in a hot gas medium, no attempts have been made to compare any of these earlier experimental results with the present theoretical model.

Recently, Lerner, Homan and Sirignano [27] have developed more advanced

new experimental techniques of measuring overall vaporization rates, droplet composition and droplet trajectories for free, isolated bicomponent paraffin droplets subject to large relative gas-droplet velocities.

The experiment consists of a monodisperse stream of droplets that is coaxially injected into a vertical, low turbulence level, heated, high speed air flow. A diagram of the experimental apparatus is shown in Figure 9.1. Heated air, produced by two ten-kilowatt electrical heaters with feedback temperature controllers, enters the stainless steel settling chamber. Ball bearings, honeycombs and screens, located downstream, provide turbulence reduction and flow straightening. A low turbulence level was confirmed via smoke injection. The large mass of the ball bearings also provides additional temperature stability. Downstream of the nozzle is the test section, a constant area pyrex tube with three flats along its length for optical access. At the entrance to the test section, a monodisperse stream of droplets, travelling at low velocity, is injected coaxially. To accomplish this, the droplet generator, surrounded by a cooling jacket, is positioned along the center line of the settling chamber and nozzle. Surrounding the end of the cooling jacket is a bluff body to prevent flow separation. The following quantities are measured along the droplet trajectory: droplet size, composition and time of flight; air temperature and velocity (axial and radial profiles). To determine droplet composition, air temperature, and air velocity, various probes are admitted through the top of the test section; the ball valve permits probe insertion without turning the air flow off. The optical table, capable of transversing the entire length of the test section, contains components used to measure droplet size. Time of flight is determined via a stroboscopic technique.¹

Since the droplet is extremely small and nonstationary, direct optical

¹This paragraph and Figure 9.1 are taken from reference [27].

observation of the droplet interior is very difficult. Hence the existence and strength of liquid internal circulation can only be tested from temporal variation of the droplet composition. A specially designed probe which separates liquid fuel droplets from a surrounding gas stream is used to measure the overall fuel composition of the droplets.

The results of this experimental study are needed for comparison with the predictions of the present theoretical model as well as two other theoretical models. Specifically, data set IV and V of [27], which are both for bicomponent fuel droplets of heptane and dodecane vaporizing at atmospheric pressure, are used for comparison here. These experimental data, in graphical form, are reproduced in Figures 9.2 - 9.9.

As shown in the figures, the ambient gas-phase temperature as well as velocity in the experiment are non-uniform along the test section. To enable the theoretical results adaptable to the experimental data for comparison, the theoretical models discussed in the previous chapters for constant ambient condition have been modified to allow the ambient condition to vary. The details are described in the next section.

9.2. Experimental Comparison Procedure

Three different liquid-phase models, namely: diffusion limit, simplified vortex and infinite diffusivity have been considered for comparison with the experimental data of [27]. In the gas phase, the simplified gas-phase model developed in Chapter 4 is used. In the infinite diffusivity model case, the formulation is similar to that in [27]. The time rate of change of droplet diameter, liquid-phase temperature, liquid-phase composition, droplet velocity and droplet distance downstream are governed by a system of first order ordinary differential equations. The details of the formulation can be found in [27] and will not be reproduced here.

A fourth order Runge-Kutta scheme is used to numerically integrate the system of equations. The initial conditions are determined from the experiment. The ambient gas-phase temperature and velocity are expressed as third order least square fits of the experimentally measured values along the test section. The ambient gas phase is assumed to be free of fuel vapor. The initial values of droplet distance and composition (assumed uniform initially) are obtained experimentally. A third order least square fit of the experimental droplet position as a function of time gives the initial values of the time and velocity. The initial droplet diameter is evaluated from a second order least square fit of the experimental droplet diameter as a function of distance downstream. Since the droplet temperature is not measurable, the initial droplet temperature is assumed to be at its wet-bulb value. This is considered to be a good approximation by Lerner et al. [27] and Talley [33]. The drag coefficient is given by the standard drag curve with the Reynolds number and other properties determined by using the one-third averaging rule.

For the diffusion-limit model and the simplified vortex model, similar solution procedure can be applied. The only exception is that the droplet temperature and species concentration are both governed by a parabolic type partial differential equation instead of a simple first order ordinary differential equation. A Crank-Nicolson type scheme is used which couples to the Runge-Kutta scheme used for the remaining coupled first order ordinary differential equations.

9.3. Results and Discussions

Two sets of bicomponent droplet data are compared. The average air velocity and temperature profiles for data set IV are shown in Figure 9.2. The experimental droplet trajectory, shown in Figure 9.3, is closely approximated by the results of all the three models. Hence, the relative gas-droplet velocity

and the droplet distance downstream are accurately predicted by all three models. The difference between the various models is so small that they practically overlap and only one curve is drawn to represent the three models.

Droplet composition versus distance downstream of the test section is plotted in Figure 9.4. Due to preferential vaporization of heptane, the more volatile component, the mass ratio of heptane to dodecane decreases as the droplet vaporizes. The infinite diffusivity model appears to significantly underpredict the mass ratio. The diffusion limit model and the vortex model are both in reasonable agreement with the experimental data. A second order least square fit of data is included in the figure. The diffusion limit model seems to be in slightly better agreement although the difference between the diffusion limit model, the vortex model and the least square fit curve is within the experimental uncertainty of the data. The underprediction of the mass ratio by the infinite diffusivity model results from overprediction of the heptane mass fraction at the droplet surface. In reality, due to large Lewis number, the more volatile heptane inside the droplet cannot diffuse fast enough to the droplet surface. This leads to a large concentration gradient near the surface. As a result, the vaporization of heptane is severely limited. Therefore, by assuming a uniform droplet composition the mass ratio will be significantly underpredicted. The experimental results suggest that the infinite diffusivity model is a poor model which gives unsatisfactory prediction for the liquid mass ratio.

The results of the droplet diameter as a function of downstream distance are shown in Figure 9.5. Approximately 16% of the droplet mass has vaporized at the exit of the test section. The experimental uncertainty of the data is as large as the difference between the different models. The infinite diffusivity model appears to underpredict the droplet diameter while the

diffusion limit model and the vortex model agree equally well with the experimental data. The underprediction of the droplet diameter by the infinite diffusivity model can be due to the overprediction of the heptane mass fraction at the liquid surface.

The results of data set V are shown in Figures 9.6 - 9.9. As indicated in Figure 9.6, both the air temperature and velocity are higher than data set IV. The vaporization rate is therefore higher for data set V. Again, the droplet trajectory is accurately predicted by all three models and the difference between the three theoretical models is so small that they practically overlap and only one curve is shown to represent the theoretical predictions of the three models.

Droplet composition versus distance downstream is plotted in Figure 9.8. As before, the infinite diffusivity model significantly underpredicts the mass ratio. Unlike in data set IV, the diffusion limit model significantly overpredicts the mass ratio. Among the three models, the vortex model appears to give the best prediction although the agreement with the data gets worse towards the end.

The results of droplet diameter as a function of downstream distance are shown in Figure 9.9. The droplet diameter decreases from about 350 μm to 310 μm and approximately 30% of the droplet mass has vaporized at the end. Again, the uncertainty of the experimental data is as large as the difference between the predictions of the various models. Both the diffusion limit model and the vortex model overpredict the droplet diameter while, on the other hand, the infinite diffusivity model agrees with the data reasonably well even though it significantly underpredicts the mass ratio.

In summary, due to large scattering in the experimental measurements,

particularly the droplet diameter, no definite conclusion can be drawn based on the experimental data.

The difference between the models at higher ambient gas temperature has been considered in chapter 6.

CHAPTER 10

CONCLUSIONS, DISCUSSIONS AND FUTURE WORK

10.1. Conclusions and Discussions

The problem of transient vaporization in a hot convective environment has been studied. A simplified liquid-phase model has been obtained which is based on the assumption of the existence of a Hill's spherical vortex inside the droplet together with some approximations made in the governing diffusion equation. A one-dimensional gas-phase model which simplifies the analysis in the gas phase through representing the heat and mass transfer rates by an optimum average for the stagnation point region and the shoulder region of a droplet has been derived. The simplification results in a one-dimensional similarity solution.

The solutions of the vaporization problem have been obtained by coupling the gas-phase similarity solution to the simplified liquid-phase solution. The resulting coupled formulation for the droplet vaporization can be expressed in the form of a parabolic partial differential equation or a Volterra type integral equation. The integral equation formulation can also be transformed into a system of coupled first-order ordinary differential equations.

The parabolic partial differential equation has been solved by a Crank-Nicolson type finite difference scheme while the system of first order ordinary differential equations are solved by Runge-Kutta method. The computational efficiencies of the two solution schemes are compared. Since the ordinary differential equation formulation eliminates the spatial dependence from the problem and therefore reduces the amount of computation, the ordinary differential equation formulation has been found to be more efficient.

The results of the coupled solutions for fuels of varying volatility in a hot atmosphere have been obtained. They are in close agreement with the results of the more detailed model developed by Prakash and Sirignano. The present simplified model predicts well the effects of the laminar gas-phase boundary layer over the droplet and the liquid internal circulation. The present model has also been examined in a spray vaporization situation. The feasibility of incorporating the present model into a one-dimensional spray vaporization calculation has been verified and the potential usefulness of the model in an overall spray situation is demonstrated. It has been found that droplet heating and vaporization are essentially unsteady. Interior droplet temperature distribution is non-uniform for a significant portion of its lifetime.

The most common vaporization models have been compared for fuels of varying volatility in a high-temperature environment. Both isolated droplet and spray vaporization have been studied. The use of the d^2 -law or infinite conductivity model has been shown to be very inadequate. For spherically-symmetric vaporization (no relative gas-droplet motion), the conduction limit model for transient heating is recommended. In practical situations where a relative gas-droplet motion exists, the simplified model of the present study is recommended when the Reynolds number based on the relative velocity is high compared to unity. The Ranz-Marshall correlation overpredicts the vaporization rate. As indicated by Sirignano [11], this type of correlation has very little theoretical justification and cannot give satisfactory results. The present study support the qualitative analysis of [11].

The spray calculations indicate an inherent unsteadiness due to the intermittent character of a spray. This unsteadiness will be interesting whenever one wishes to resolve structure on the scale of the average distance between droplets.

The simplified analysis developed for the single-component droplet has been extended to the multicomponent droplet case. The solutions for a heptane dodecane bicomponent droplet case vaporizing in a hot atmosphere have been obtained. The results have been compared with the results of the infinite diffusivity model and the spherical diffusion limit model.

It has been found that due to neglect of the thermal and mass diffusion resistances, there are substantial differences in the vaporization behaviors between the infinite diffusivity model and the other two models. At short times, the disagreements between the various models are caused by the difference in the mode of thermal energy transfer; while for the bulk of the droplet lifetime, the discrepancies are mainly due to the differences in the mass diffusion models. The disagreements between the vortex model and the diffusion limit model have been found to be relatively less.

The effects of different gas-phase models and initial droplet mixture composition on the vaporization behaviors of a heptane dodecane bicomponent droplet have also been examined. Considerable discrepancies in vaporization behaviors have been found between the present simplified gas-phase model and the Ranz-Marshall correlation. The disagreements worsen as the ambient temperature increases.

As in the single component droplet case, the spherical diffusion limit model for transient diffusion is recommended for stagnant situation (no relative gas-droplet motion). In practical convective situations, the present simplified model is recommended for high Reynolds Number case. The Ranz-Marshall correlation, which overpredicts the vaporization, is not satisfactory for the transient vaporization problem.

The vaporization characteristics of a droplet, except for the initial period, is

dominated by the heavier component. The larger the initial composition of the lighter component, the more it resembles the pure light component.

Attempts have been made to compare the results of the present models as well as the diffusion limit model and the infinite diffusivity model with experimental data. Due to large scattering in the experimental measurements, no definite conclusions can be drawn based on the experimental data.

10.2. Future Work

Since the objective of the present study is to develop a simplified algorithm for the droplet vaporization, various complexities have been omitted from the present model. Phenomena such as droplet interactions within a spray, liquid-phase chemical reactions and droplet interactions within a turbulent gas field are very important in many practical situations. These are considered to be useful research problems for future study.

While the detailed model developed by Prakash and Sirignano is too cumbersome to be included in a complete spray vaporization situation, the present simplified model should be more useful.

Tal (Thau) *et al* [43-47] have recently studied the hydrodynamics and heat transfer in an array of droplets. It would be useful to examine the results of inserting the present simplified model into their analysis.

It has been demonstrated that [35, 36], the entrapment of the volatile components within the more rapidly heated droplet interior may lead to the initiation of either homogeneous or heterogeneous nucleation. This can result in the fragmentation of the droplet due to the internal pressure buildup. The present model would be useful in predicting induction time for droplet vaporization explosion of a multicomponent droplet.

The present simplified model is for high (compared to unity) Reynolds number situation. Low Reynolds number case is an area for future work.

Finally, an approach which uses the more exact analysis developed by Prakash and Sirignano in a parametric study to generate a suitable correlation between burning rate, pressure, ambient oxidizer concentration, internal circulation, etc. appears to be a possible alternative useful for comprehensive spray models. Although the fact that the problem is basically transient in nature may introduce complexities to the correlation scheme, someone should be encouraged to do it.

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APPENDIX A

COUPLED GAS-LIQUID SOLUTION IN THE NON-VAPORIZING DROPLET CASE I - INTEGRAL EQUATION SOLUTION

In the non-vaporizing case, the Nusselt number is a function of Reynolds number, but independent of temperature so that, for our purposes, it may be considered to be constant with time. It can be shown that the temperature gradient at the droplet surface is given by

$$\frac{\partial T}{\partial \phi} = A + B T_s \quad (\text{A.1})$$

where

$$A = \frac{Nu}{8} \left(\frac{k_g}{k_l} \right) T_\infty \quad (\text{A.2})$$

and

$$B = \frac{Nu}{8} \left(\frac{k_g}{k_l} \right) \quad (\text{A.3})$$

The solution for the non-vaporizing droplet with time-varying temperature gradient boundary condition $\partial T / \partial \phi = f(r)$ is given by

$$T(\tau, \phi) = \left[\phi - \frac{1}{2} - 4 \sum_{n=1}^{\infty} \frac{J_0(\lambda_n \phi^{1/2})}{\lambda_n^2 J_0(\lambda_n)} \right] f(\tau) \quad (A.4)$$

$$+ \int_0^{\tau} f(x) dx + \sum_{n=1}^{\infty} \left[\frac{J_0(\lambda_n \phi^{1/2})}{J_0(\lambda_n)} \int_0^{\tau} f(\tau) \exp(-\lambda_n^2(\tau-x)/4) dx \right]$$

Substituting (A.1) for $f(\tau)$ and evaluating at $\phi=1$ the surface temperature after some algebraic manipulation is governed by

$$T_s(\tau) = g(\tau) + \int_0^{\tau} K(\tau-x) T_s(x) dx \quad (A.5)$$

which is a linear Volterra Integral Equation of the second kind.

where

$$g(\tau) = A \left[\tau + \frac{1}{2} - 4 \sum_{n=1}^{\infty} \frac{\exp(-\lambda_n^2 \tau/4)}{\lambda_n^2} \right] \quad (A.6)$$

and

$$K(\tau-x) = B \left[1 + \sum_{n=1}^{\infty} \exp(-\lambda_n^2(\tau-x)/4) \right] \quad (A.7)$$

The solution of the integral equation (A.5) can be obtained readily by means of product integration method as suggested in [31] and [32]. The surface temperature T_s can be generated from the following recurrence formula.

$$\frac{g(h)}{1-i_1(1)} \quad n=1$$

$$T(nh) =$$

$$\left(g(nh) + \sum_{k=1}^{N-1} A(k)T[(n-k)h] \right) / (1 - i_1(1)) \quad n > 1 \quad (\text{A.8})$$

where

$$A(k) = i_0(k) + i_1(k+1) - i_1(k) \quad (\text{A.9})$$

$$i_0(k) = B[h + 4(S_1(k-1) - S_1(k))] \quad (\text{A.10})$$

$$i_1(k) = B\left[\frac{h}{2} + 4 S_1(k-1) - \frac{4}{h} (S_2(k-1) - S_2(k))\right] \quad (\text{A.11})$$

$$S_1(k) = \sum_{n=1}^{\infty} \frac{\exp(-\lambda_n^2 kh/4)}{\lambda_n^2} \quad (\text{A.12})$$

$$S_2(k) = \sum_{n=1}^{\infty} \frac{\exp(-\lambda_n^2 kh/4)}{\lambda_n^4} \quad (\text{A.13})$$

The result for surface temperature in a case when $A = 2.4842$ and $B = -0.4933$ is presented in Figure A.1. As expected, surface temperature increases with time due to droplet heating. The comparison with a finite-difference calculation using exact g_1 and g_2 values is shown in the same figure to be very favorable. A finite-difference calculation employing the approximate g_1 and g_2 values resulted in differences with the integral equation solution that could not be detected graphically. Once the surface temperature is known, Equation (A.1) may be utilized to determine the gradient at the surface and, therefore, the heat flux as functions of time. Now, (A.4) would yield the behavior of the temperature in the droplet interior.

APPENDIX B

SOURCE/SINK TERMS IN THE GAS-PHASE EQUATIONS OF THE ONE-DIMENSIONAL SPRAY VAPORIZATION FORMULATION

The source/sink terms in the gas-phase equations (1, 2) are given as follows:

$$S_{\rho} = \frac{t_r}{L_r} \frac{1}{\Delta x} \sum_k m_k n_k \quad (B.1)$$

$$S_{Y_f} = \frac{1}{\rho} S_{\rho} (1 - Y_f) \quad (B.2)$$

$$S_{Y_o} = - \frac{1}{\rho} S_{\rho} Y_o \quad (B.3)$$

$$S_{\phi} = - \frac{S_{\rho}}{\rho p \gamma - 1} \{ H + T_r - T_k \} \quad (B.4)$$

$$m_k = 4 \pi r_k \mu (1 + 0.3 Re_k^{0.5}) \ln(1 + B_k) \quad (B.5)$$

for Ranz-Marshall Correlation

$$= 4 \pi r_k \mu \left\{ \frac{2}{\pi} Re_k \right\}^{0.5} f(B_k)$$

for the present simplified model

$$B_k = \frac{T - T_k}{H} \quad (B.6)$$

$$H = \frac{(1 - Y_{fs})(T - T_k)}{Y_{fs} - Y_f} \quad (B.7)$$

$$Y_{fs}^{-1} = 1 + \frac{M_a'}{M_f'} (x_{fs}^{-1} - 1) \quad (B.8)$$

$$x_{fs} = \frac{p_n'}{p'} \exp \left[\frac{L' M_f'}{R'} \left(\frac{1}{T_{bn}'} - \frac{1}{T_k} \right) \right] \quad (B.9)$$

In the above relations, S_{Yf} and S_{Yo} are the source and sink terms for the fuel vapor and oxidizer mass fractions, x_{fs} is the mole fraction at the droplet surface, M_a' is the molecular weight of the gas-phase (excluding fuel vapor), T_{bn}' is the liquid fuel boiling temperature at the normal pressure p_n' , p is the prevailing pressure, and Σ represents the summation over all droplet groups which happen to be in a given gas-phase mesh, of size Δx . A phase equilibrium assumption has been made at the droplet surface and Clausius-Clapeyron relation has been used. The different methods of computing the droplet surface temperature T_k distinguish the various liquid phase models examined in the present spray problem.

APPENDIX C

COUPLED GAS-LIQUID SOLUTION IN THE NON- VAPORIZING DROPLET CASE II - SERIES SOLUTION

It was shown in Appendix A that the surface temperature of a non-vaporizing droplet is governed by the following integral equation:

$$T_s(\tau) = f(\tau) + \int_0^\tau K(\tau-x)T_s(x)dx \quad (C.1)$$

where

$$f(\tau) = A \left[\tau + \frac{1}{2} - 4 \sum_{n=1}^{\infty} \frac{e^{-\lambda_n^2 \tau/4}}{\lambda_n^2} \right] \quad (C.2)$$

and

$$K(\tau-x) = B \left[1 + \sum_{n=1}^{\infty} e^{-\lambda_n^2 (\tau-x)/4} \right] \quad (C.3)$$

By defining,

$$g_0(\tau) \equiv B \int_0^\tau T_s(x) dx \quad (C.4)$$

and

$$g_n(\tau) \equiv B \int_0^\tau e^{-\lambda_n^2 (\tau-x)/4} T_s(x) dx$$

$$= \frac{4A}{\lambda_n^2} e^{-\lambda_n^2 \tau/4}; \text{ for } n \geq 1 \quad (C.5)$$

(C.1) can be written as

$$T_s(\tau) = A(\tau^{1/2}) + \sum_{n=1}^{\infty} g_n(\tau) \quad (C.6)$$

Taking the τ derivative of g_i 's gives

$$\frac{dg_0}{d\tau} = B T_s(\tau) \quad (C.7)$$

$$\frac{dg_n}{d\tau} = B T_s(\tau) - \frac{\lambda_n^2}{4} g_n(\tau); n \geq 1 \quad (C.8)$$

Also, at $\tau = 0$

$$g_0(0) = 0 \quad (C.9)$$

$$g_n(0) = -\frac{4A}{\lambda_n^2}; n \geq 1 \quad (C.10)$$

and

$$T_s(0) = 0. \quad (C.11)$$

Therefore the integral equation formulation is converted into a system of first order ordinary differential equations, (C.7) and (C.8), together with the associated initial conditions, (C.9), (C.10), and (C.11).

Equations (C.7) and (C.8) can also be written a matrix form as

$$[G]' = B[M] [G] + [Q] \quad (C.12)$$

where $[]$ denotes matrix and prime denotes τ derivatives and

$$[G] = [g_i]^T = [g_0, g_1, \dots, g_N]^T \quad (C.13)$$

$$[M] = [m_{ij}]; m_{ij} = 1 - \frac{\lambda_i^2}{4B} ; \text{ for } i=j \neq 0$$

$$= 1 ; \text{ otherwise} \quad (C.14)$$

$$[Q] = [q_i] ; q_i = BA(\tau + 1/2) \quad (C.15)$$

Here only a finite number of g 's will be considered. Note that $[Q]$ is actually a constant vector.

$[M]$ can be diagonalized as

$$[M] = [P]^{-1}[\Lambda][P] \quad (C.16)$$

by defining

$$[\Lambda] = [\Lambda_{ij}] ; \Lambda_{ii} = \text{eigenvalues of } [M]$$

$$\Lambda_{ij} = 0 ; i \neq j \quad (C.17)$$

and

$$[P] = [P_{ij}] ; P_{ij} = j^{\text{th}} \text{ component of the } i_{\text{th}}$$

$$\text{eigenvector of } [M] \quad (C.18)$$

Note that $[P]$ ($[P]^{-1}$) stores the eigenvectors of $[M]$ by rows (columns).

Substituting (C.16) into (C.12) gives

$$[G]' = B[P]^{-1}[\Lambda][P][G] + [Q] \quad (C.19)$$

which can be written as

$$[W]' = [D][W] + [R] \quad (C.20)$$

where

$$[W] = [w_i] = [P][G] \quad (C.21)$$

$$[D] = [d_{ii}] = B[\Lambda] \quad (C.22)$$

$$[R] = [r_i] = [P][Q] \quad (C.23)$$

In (C.22), [D] is a diagonal matrix. Note that now w_i 's are decoupled and for each w_i , we have

$$w_i' = d_i w_i + r_i \quad (C.24)$$

whose solution is given by

$$w_i(\tau) = e^{d_i \tau} \int_0^\tau e^{-d_i x} r_i(x) dx + w_i(0) e^{d_i \tau} \quad (C.25)$$

From (C.23),

$$r_i = s_i BA(\tau + 1/2) \quad (C.26)$$

where s_i is the sum of all the components of the i^{th} eigenvector of [M].

From (C.21)

$$\begin{aligned}
 w_i(o) &= [V_i]^T [G] \big|_{\tau=0} \\
 &= \sum_j v_i^j g_j(o)
 \end{aligned} \tag{C.27}$$

where V_i is the i^{th} eigenvector of $[M]$ and v_i^j is the j^{th} component of V_i .

Upon substitution of (C.26) and (C.27) into (C.25), we obtain:

$$w_i = a_i e^{d_i \tau} + \beta_i \tau + \gamma_i \tag{C.28}$$

where

$$a_i = \left(\sum_j v_i^j g_j(o) \right) - \gamma_i \tag{C.29}$$

$$\beta_i = -BA \, s_i / d_i \tag{C.30}$$

$$\gamma_i = \left(\frac{1}{2} + \frac{1}{d_i} \right) \beta_i \tag{C.31}$$

Using (C.21) to transform w_i back to g_i yields

$$\begin{aligned}
 g_j &= \sum_i v_i^j w_i \\
 &= \sum_i v_i^j (a_i e^{d_i \tau} + \beta_i \tau + \gamma_i) \\
 &= \left(\sum_i v_i^j a_i e^{d_i \tau} \right) + \sum_i v_i^j \beta_i \tau \\
 &\quad + \sum_i v_i^j \gamma_i
 \end{aligned} \tag{C.32}$$

Finally, substituting (C.32) into (C.6) gives

$$T_s(\tau) = (A + \sum_i s_i \beta_i) \tau + \left(\frac{A}{2} + \sum_i s_i \gamma_i\right) + \sum_i a_i s_i e^{d_i \tau} \quad (C.33)$$

Note that the terms in parenthesis are constants. Therefore $T_s(\tau)$ can be written in the following form

$$T(\tau) = C_1 \tau + C_2 + \sum_i a_i e^{d_i \tau} \quad (C.34)$$

where

$$C_1 = A + \sum_i s_i \beta_i$$

$$C_2 = \frac{A}{2} + \sum_i s_i \gamma_i \quad (C.35)$$

and

$$a_i = a_i s_i$$

The results for the case where $A = 2.4842$ and $B = -0.4933$ have been obtained and are in agreement with the results obtained in Appendix A. The values of C_1 , C_2 and the first 10 a_i 's and d_i 's are given below

$$C_1 \approx 0$$

$$C_2 \approx 5.04$$

and

a_i	d_i
3.9186	- 0.3913
0.5667	- 4.1561
0.1910	- 12.7967
0.0937	- 26.3689
0.0553	- 44.8745
0.0364	- 68.3171
0.0257	- 96.6917
0.0192	- 129.9994
0.0148	- 168.2449
0.0118	- 211.4235

APPENDIX D

SERIES SOLUTIONS FOR THE UNCOUPLED LIQUID-PHASE THERMAL DIFFUSION EQUATION WITH ZERO C

Consider the following partial differential equation

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + \frac{\partial T}{\partial \phi} ; 0 \leq \phi \leq \phi_0 \quad (D.1)$$

together with the initial and boundary conditions

$$(i) \quad \text{at } \tau = 0, T = 0$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial T}{\partial \tau} = \frac{\partial T}{\partial \phi}$$

$$(iiia) \quad \text{at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = 1$$

or

$$(iiib) \quad \text{at } \phi = \phi_0, T = 1 \quad (D.2)$$

where (iiia) corresponds to the unity temperature gradient boundary condition case and (iiib) corresponds to the unity temperature boundary condition case. The solutions for both cases are presented here.

Unity temperature boundary condition:

Taking the Laplace Transform of Equations (D.1) and (D.2) on τ gives

$$\phi \frac{d^2 T}{d\phi^2} + \frac{dT}{d\phi} - ST = 0 \quad (D.3)$$

and

$$\begin{aligned} \text{(i) at } \phi = 0, ST(S, 0) &= \frac{dT(S, 0)}{d\phi} \\ \text{(ii) at } \phi = \phi_0, T(S, \phi_0) &= \frac{1}{S} \end{aligned} \quad (D.4)$$

where S is the variable of the Laplace Transform. The general solution for Equation (D.3) is given by [40].

$$T = A J_0(i2(S\phi)^{1/2}) + B Y_0(i2(S\phi)^{1/2}) \quad (D.5)$$

where A and B are constants and J_0 , Y_0 are Bessel functions. Since T is finite, B must vanish. Hence

$$T = A J_0(i2(S\phi)^{1/2}) \quad (D.6)$$

Substituting (D.6) into (ii) of (D.4) yields

$$A = \frac{1}{S J_0(i2(S\phi_0)^{1/2})} \quad (D.7)$$

Therefore,

$$T(S, \phi) = \frac{J_0(i2(S\phi)^{1/2})}{S J_0(i2(S\phi_0)^{1/2})} \quad (D.8)$$

It can be shown readily that (i) of (D.4) is satisfied by (D.8).

By the Inversion Integral Technique,

$$T(\tau, \phi) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{S\tau} J_0(i2(S\phi)^{1/2})}{S J_0(i2(S\phi_0)^{1/2})} dS \quad (D.9)$$

Now $J_0(i2(S\phi_0)^{1/2})$ has simple zeros where $i2(S\phi_0)^{1/2} = \lambda_1, \lambda_2, \dots, \lambda_n$, and $J_0(\lambda_n) = 0$. Thus the integrand has simple poles at $S = -\lambda_n^2/4\phi_0$, $n = 1, 2, 3, \dots$ and also at $S = 0$. By using the method of residues, we have:

Residue, R_0 , of integrand at $S = 0$:

$$R_0 = \lim_{S \rightarrow 0} \frac{e^{S\tau} J_0(i2(S\phi)^{1/2})}{J_0(i2(S\phi_0)^{1/2})} = 1 \quad (D.10)$$

Residue, R_n , of integrand at $S = S_n = -\lambda_n^2/4\phi_0$

$$R_n = \lim_{S \rightarrow S_n} \frac{(S-S_n) e^{S\tau} J_0(i2(S\phi)^{1/2})}{S J_0(i2(S\phi_0)^{1/2})} \quad (D.11)$$

$$= \lim_{S \rightarrow S_n} \frac{(S-S_n)}{J_0(i2(S\phi_0)^{1/2})} \cdot \lim_{S \rightarrow S_n} \frac{e^{S\tau} J_0(i2(S\phi)^{1/2})}{S}$$

$$= \frac{e^{S_n \tau} J_0(i2(S_n \phi)^{1/2})}{i(\phi_0 S_n)^{1/2} J_1(i2(S_n \phi_0)^{1/2})} \quad (D.12)$$

where L' Hospital rule has been used in obtaining the first limit and also $J_0'(x) = J_1(x)$. Here superscript prime denotes derivative. Then

$$T(\tau, \phi) = \sum_{n=1}^{\infty} R_n$$

$$= 1 - \sum_{n=1}^{\infty} \frac{2}{\lambda_n} \frac{J_0(\lambda_n(\phi/\phi_0)^{1/2})}{J_1(\lambda_n)} e^{-(\lambda_n^2 \tau / 4 \phi_0)} \quad (D.13)$$

Unity temperature gradient boundary condition:

The boundary condition (ii) of (D.4) becomes

$$\frac{d\tau(S, \phi_0)}{d\phi} = \frac{1}{S} \quad (D.14)$$

Substituting (D.6) into (D.14) yields

$$A = \frac{i \phi_0^{1/2}}{S^{3/2} J_1(i2(S\phi_0)^{1/2})} \quad (D.15)$$

Therefore,

$$T(S, \phi) = \frac{i \phi_0^{1/2} J_0(i2(S\phi)^{1/2})}{S^{3/2} J_1(i2(S\phi_0)^{1/2})} \quad (D.16)$$

By the Inversion Integral Technique,

$$T(\tau, \phi) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{i \phi_0^{1/2} J_0(i2(S\phi)^{1/2}) e^{S\tau}}{S^{3/2} J_1(i2(S\phi_0)^{1/2})} dS \quad (D.17)$$

Now $J_1(i2(S\phi_0)^{1/2})$ has simple zeros where $i2(S\phi_0)^{1/2} = \lambda_1, \lambda_2, \dots, \lambda_n, \dots$ and $J_1(\lambda_n) = 0$. Thus the integrand has simple poles at $S = -\lambda_n^2/4\phi_0$, $n = 1, 2, 3, \dots$

Expanding $J_1(i2(S\phi_0)^{1/2})$ gives:

$$J_1(i2(S\phi_o)^{1/2}) = i(S\phi_o)^{1/2} - \frac{(i(S\phi_o)^{1/2})^3}{2} + O(S^{5/2}) \quad (D.18)$$

The denominator of the integrand can be expanded as

$$S^{3/2} J_1(i2(S\phi_o)^{1/2}) = i\phi_o^{1/2} S^2(1 + \frac{\phi_o}{2}S + O(S^2)) \quad (D.19)$$

Therefore $S = 0$ is actually a double pole. Again by using the method of residues, we have:

Residue, R_n , of integrand at $S = S_n = -\lambda_n^2/4\phi_o$ is:

$$R_n = \lim_{S \rightarrow S_n} \frac{(S-S_n) i\phi_o^{1/2} e^{S\tau} J_o(i2(S\phi_o)^{1/2})}{S^{3/2} J_1(i2(S\phi_o)^{1/2})} \quad (D.20)$$

$$\begin{aligned} &= \lim_{S \rightarrow S_n} \frac{(S-S_n)}{J_1(i2(S\phi_o)^{1/2})} \cdot \lim_{S \rightarrow S_n} \frac{i\phi_o^{1/2} e^{S\tau} J_o(i2(S\phi_o)^{1/2})}{S^{3/2}} \\ &= -\frac{4\phi_o}{\lambda_n^2} \frac{J_o(\lambda_n(\phi/\phi_o)^{1/2})}{J_1'(\lambda_n)} \exp(-(\lambda_n^2 \tau/4\phi_o)) \end{aligned} \quad (D.21)$$

where L' Hospital rule has again been used in obtaining the first limit. Here superscript prime denotes derivative.

Residue, R_o , of integrand at $S = 0$ is:

From [41], R_o is given by

$$R_o = \lim_{S \rightarrow 0} \left(\frac{2p'(o)}{q''(o)} - \frac{2p(o)q'''(o)}{3[q''(o)]^2} \right) \quad (D.22)$$

where $p(s)$ and $q(s)$ are the numerator and the denominator of the integrand, respectively. The superscript prime denotes derivatives. It can be shown easily that

$$\begin{aligned}
 \text{(i)} \quad p(o) &= i (\phi_o)^{1/2} \\
 \text{(ii)} \quad p'(o) &= i (\phi_o)^{1/2} (\phi + \tau) \\
 \text{(iii)} \quad q''(o) &= i 2 (\phi_o)^{1/2} \\
 \text{(iv)} \quad q'''(o) &= i 3 \phi_o^{3/2}
 \end{aligned} \tag{D.23}$$

Substituting (D.23) into (D.22) gives,

$$R_o = \phi + \tau - \frac{\phi_o}{2} \tag{D.24}$$

Now,

$$\begin{aligned}
 T(\tau, \phi) &= \sum_{n=0}^{\infty} R_n \\
 &= \phi - \frac{\phi_o}{2} + \tau - 4\phi_o \sum_{n=1}^{\infty} \frac{e^{-(\lambda_n^2 \tau / 4 \phi_o)} J_o(\lambda_n (\phi / \phi_o)^{1/2})}{\lambda_n^2 J_1'(\lambda_n)}
 \end{aligned} \tag{D.25}$$

APPENDIX E

SERIES SOLUTIONS FOR THE UNCOUPLED LIQUID-PHASE THERMAL DIFFUSION EQUATION WITH CONSTANT C

Consider the following partial differential equation

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + (1 + C\phi) \frac{\partial T}{\partial \phi} ; 0 \leq \phi \leq \phi_0 \quad (\text{E.1})$$

together with the initial and boundary conditions given by

$$(i) \quad \text{at } \tau = 0, T = 0$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$$

$$(iiia) \quad \text{at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = 1 \quad (\text{E.2})$$

or

$$(iiib) \quad \text{at } \phi = \phi_0, T = 1$$

C is a constant in Equation (E.1). In the boundary condition, (iiia) represents the unity temperature gradient boundary condition case and (iiib) corresponds to the unity temperature boundary condition case. The solutions for both cases are presented in this appendix.

Unity temperature boundary condition:

Taking the Laplace Transform of Equations (E.1) and (E.2) on τ gives

$$\phi \frac{d^2 T}{d\phi^2} + (1+C\phi) \frac{dT}{d\phi} - ST = 0 \quad (E.3)$$

and

$$\begin{aligned} \text{(i) at } \phi = 0, ST(S,0) &= \frac{dT(S,0)}{d\phi} \\ \text{(ii) at } \phi = \phi_0, T(S,\phi_0) &= \frac{1}{S} \end{aligned} \quad (E.4)$$

where S is the variable in the Laplace Transform.

Since $\phi = 0$ is a regular singular point in Equation (E.3), the method of Frobenius is used to obtain the series solutions. Assuming a series solution of the form

$$T = \sum_{k=0}^{\infty} A_k \phi^{k+a} \quad (E.5)$$

with the exponent a and all the coefficients A_k still undetermined. By differentiating twice, we have

$$\frac{dT}{d\phi} = \sum_{k=0}^{\infty} (k+a) A_k \phi^{(k+a-1)} \quad (E.6)$$

and

$$\frac{d^2 T}{d\phi^2} = \sum_{k=0}^{\infty} (k+a)(k+a-1) A_k \phi^{(k+a-2)} \quad (E.7)$$

Substituting Equations (E.5), (E.6), and (E.7) into Equation (E.3) gives

$$\begin{aligned} & \sum_{k=0}^{\infty} (k+a)(k+a-1)A_k \phi^{(k+a-1)} + \sum_{k=0}^{\infty} (k+a)A_k \phi^{(k+a-1)} \\ & + \sum_{k=0}^{\infty} (k+a)C A_k \phi^{(k+a)} - S \sum_{k=0}^{\infty} A_k \phi^{(k+a)} = 0 \end{aligned} \quad (E.8)$$

After rearranging terms, it becomes

$$a^2 A_0 \phi^{(a-1)} + \sum_{k=0}^{\infty} [(k+a+1)^2 A_{k+1} - (S-(k+a)C)A_k] \phi^{(k+a)} = 0 \quad (E.9)$$

The uniqueness of power series requires that the coefficients of each power of ϕ on the left-hand side of Equation (E.9) must vanish individually. The requirement that the coefficient of $\phi^{(a+1)}$ vanish yields

$$a^2 A_0 = 0 \quad (E.10)$$

Since A_0 had been chosen as the coefficient of the lowest nonvanishing term of the series, Equation (E.4), hence, by definition, $A_0 \neq 0$. Therefore, we have

$$a^2 = 0 \quad (E.11)$$

which implies that $a = 0$.

The requirement that the coefficient of $\phi^{(k+a)}$ ($k \geq 0$) vanish gives,

$$[(k+a+1)^2 A_{k+1} - (S-(k+a)C)A_k] = 0 \quad (E.12)$$

with $a = 0$, it becomes

$$A_{k+1} = \frac{(S-kC)}{(k+1)^2} A_k \quad (E.13)$$

which is a two-term recurrence relation. Given A_0 , A_1 can be computed and then A_2 , A_3 , and so on up as far as desired. It can be shown readily that

$$A_{k+1} = \frac{(S-kC)(S-(k-1)C)\dots(S-C)S}{(k+1)!^2} \quad (E.14)$$

Here since the two roots of the indicial equation (i.e. Equation (E.11)) are equal, only one solution can be obtained by the present series substitution method. The other independent series solution of T will be singular at $\phi = 0$ and since T is finite there, no attempt is made to seek that second solution.

Hence,

$$T(S, \phi) = A_0 F(S, C, \phi) \quad (E.15)$$

where, for brevity,

$$F(S, C, \phi) \equiv \left[1 + \sum_{k=1}^{\infty} \frac{S(S-C)\dots(S-(k-1)C)}{(k!)^2} \phi^k \right] \quad (E.16)$$

Substituting (E.15) into (ii) of (E.4) gives,

$$A_0 = \frac{1}{SF(S, C, \phi_0)} \quad (E.17)$$

Therefore,

$$T(S, \phi) = \frac{F(S, C, \phi)}{SF(S, C, \phi_0)} \quad (E.18)$$

It can be verified easily that (i) of (E.4) is satisfied by Equation (E.15).

By the Inversion Integral Technique,

$$T(\tau, \phi) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{S\tau} T(S, \phi) dS \quad (E.19)$$

$$= \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{S\tau} F(S, C, \phi)}{SF(S, C, \phi_0)} dS \quad (E.20)$$

Now $F(S, C, \phi_0)$ has simple zeros, S_n , where $F(S_n, C, \phi_0) = 0$. Thus the integrand has simple poles at $S = S_n$ and also at $S = 0$. By using the method of residues, we have:

Residue, R_0 , of integrand at $S = 0$:

$$R_0 = \lim_{S \rightarrow 0} \frac{e^{S\tau} F(S, C, \phi)}{F(S, C, \phi_0)} = 1 \quad (E.21)$$

Residue, R_n , of integrand at $S = S_n$:

$$R_n = \lim_{S \rightarrow S_n} \frac{(S - S_n) e^{S\tau} F(S, C, \phi)}{SF(S, C, \phi_0)} \quad (E.22)$$

$$\begin{aligned} &= \lim_{S \rightarrow S_n} \frac{(S - S_n)}{F(S, C, \phi_0)} \cdot \lim_{S \rightarrow S_n} \frac{e^{S\tau} F(S, C, \phi)}{S} \\ &= \frac{e^{S_n \tau} F(S_n, C, \phi)}{S_n F_S(S_n, C, \phi_0)} \end{aligned} \quad (E.23)$$

where L' Hospital rule has been used in obtaining the first limit and F_S denotes partial derivative of F with respect to S . Then

$$\begin{aligned}
 T(\tau, \phi) &= \sum_{n=0}^{\infty} R_n \\
 &= 1 + \sum_{n=0}^{\infty} \frac{e^{S_n \tau} F(S_n, C, \phi)}{S_n F(S_n, C, \phi_0)}
 \end{aligned} \tag{E.24}$$

Unity temperature gradient boundary condition:

In this case, the boundary condition (ii) of (E.4) is replaced by

$$\frac{dT(S, \phi_0)}{d\phi} = \frac{1}{S} \tag{E.25}$$

Substituting (E.15) into (E.25) yields

$$A_0 \left. \frac{\partial F}{\partial \phi} \right|_{\phi=\phi_0} = \frac{1}{S} \tag{E.26}$$

For brevity, let G be $\partial F / \partial \phi$, then

$$G(S, C, \phi) = \sum_{k=1}^{\infty} \frac{S(S-C) \dots (S-(k-1)C)}{k(k-1)!^2} \phi^{k+1} \tag{E.27}$$

and

$$A_0 = \frac{1}{SG(S, C, \phi_0)} \tag{E.28}$$

Therefore,

$$T(S, \phi) = \frac{F(S, C, \phi)}{SG(S, C, \phi_0)} \tag{E.29}$$

By the Inversion Integral Technique,

$$T(\tau, \phi) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{S\tau} F(S, C, \phi)}{SG(S, C, \phi_0)} dS \quad (E.30)$$

Now $G(S, C, \phi_0)$ has simple zeros, S_n , where $G(S_n, C, \phi_0) = 0$. Thus the integrand has simple poles at $S = S_n$; $n \geq 1$.

Expanding $G(S, C, \phi_0)$ gives

$$G(S, C, \phi_0) = S + \frac{S(S-C)}{2} \phi_0 + \dots \quad (E.31)$$

Therefore $SG(S, C, \phi_0)$ has a double root at $S = 0$. Again by using the method of residues, we have

Residue, R_n , of integrand at $S = S_n$; $n \geq 1$

$$R_n = \lim_{S \rightarrow S_n} \frac{(S-S_n) e^{S\tau} F(S, C, \phi)}{S G(S, C, \phi_0)} \quad (E.32)$$

$$= \lim_{S \rightarrow S_n} \frac{(S-S_n)}{G(S, C, \phi_0)} \cdot \lim_{S \rightarrow S_n} \frac{e^{S\tau} F(S, C, \phi)}{S}$$

$$= \frac{e^{S_n \tau} F(S_n, C, \phi)}{S_n G_S(S_n, C, \phi_0)} \quad (E.33)$$

where L' Hospital rule has again been used in obtaining the first limit and G_S denotes partial derivatives of G with respect to S .

Residue, R_0 , of integrand at $S = 0$:

From [41], R_o is given by

$$R_o = \lim_{S \rightarrow 0} \left[\frac{2p'(S)}{q''(S)} - \frac{2}{3} \frac{p(S)q'''(S)}{[q''(S)]^2} \right] \quad (E.34)$$

where $p(s)$ and $q(s)$ are the numerator and the denominator of the integrand respectively. The primes denote derivatives. It can be shown that

$$\begin{aligned} (i) \quad & p(o) = 1 \\ (ii) \quad & q'(o) = \tau + F_S(o, C, \phi) \\ (iii) \quad & q''(o) = 2G_S(o, C, \phi_o) \\ (iv) \quad & q'''(o) = 3G_{SS}(o, C, \phi_o) \end{aligned} \quad (E.35)$$

Here subscript S denote partial derivative with respect to S. Substituting (E.35) into (E.34) gives

$$R_o = \frac{\tau + F_S(o, C, \phi)}{G_S(o, C, \phi_o)} - \frac{1}{2} \frac{G_{SS}(o, C, \phi_o)}{G_S^2(o, C, \phi_o)} \quad (E.36)$$

Now,

$$\begin{aligned} T(\tau, \phi) &= \sum_{n=0}^{\infty} R_n \\ &= \frac{\tau + F_S(o, C, \phi)}{G_S(o, C, \phi_o)} - \frac{1}{2} \frac{G_{SS}(o, C, \phi_o)}{G_S^2(o, C, \phi_o)} \\ &\quad + \sum_{n=1}^{\infty} \frac{e^{S_n \tau} F(S_n, C, \phi)}{S_n G_S(S_n, C, \phi_o)} \end{aligned} \quad (E.37)$$

A summary of the functions generated in this appendix is given below

$$F(S, C, \phi) = \sum_{k=1}^{\infty} \frac{S(S-C)\dots(S-(k-1)C)\phi^k}{(k!)^2}$$

$$G(S, C, \phi) = \sum_{k=1}^{\infty} \frac{S(S-C)\dots(S-(k-1)C)\phi^{k-1}}{k((k-1)!)^2}$$

$$F_S(S, C, \phi) = \sum_{k=0}^{\infty} \frac{(-1)^k C^k \phi^{(k+1)}}{(k+1)(k+1)!}$$

$$G_S(S, C, \phi) = \sum_{k=0}^{\infty} \frac{(-k)^k C^k \phi^k}{(k+1)!}$$

$$G_{SS}(0, C, \phi) = \sum_{k=1}^{\infty} \frac{2(-1)^{(k-1)} a_k C^{(k-1)} \phi^k}{(k+1)(k!)^2}$$

where $a_k = k a_{k-1} + (k-1)!$; $k \geq 2$ and $a_1 = 1$.

It can be shown that the results of Appendix D can be obtained from the results of this appendix simply by letting $C = 0$.

APPENDIX F

VARIABLE TRANSFORMATION FOR THE UNCOUPLED LIQUID-PHASE THERMAL DIFFUSION EQUATION WITH TIME VARYING COEFFICIENT C

For the vaporizing droplet case, the temperature inside the droplet is governed by

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + [1 + C(\tau)\phi] \frac{\partial T}{\partial \phi}; \quad 0 \leq \phi \leq \phi_0 \quad (F.1)$$

together with the following initial and boundary conditions.

$$(i) \quad \text{at } \tau = 0, T = 0$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$$

$$(iii) \quad \text{at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = q(\tau) \quad (F.2)$$

Equation (F.1) has a time varying coefficient for the $\partial T / \partial \phi$ term which eliminates the possibility of any analytic solutions. Variable transformations are sought which can convert Equation (F.1) into a differential equation with only time-invariant coefficients at the expense of $C(\tau)$ being approximated by a certain functional form only.

The following transformation on T is considered.

$$V = Te^{-h}$$

(F.3)

where V and h are functions of both r and ϕ . Then,

$$(i) \quad \frac{\partial V}{\partial r} = \frac{\partial V}{\partial r} e^h + \frac{\partial h}{\partial r} V e^h$$

$$(ii) \quad \frac{\partial T}{\partial \phi} = \frac{\partial V}{\partial \phi} e^h + \frac{\partial h}{\partial \phi} V e^h$$

$$(iii) \quad \frac{\partial^2 T}{\partial \phi^2} = \frac{\partial^2 V}{\partial \phi^2} e^h + 2 \frac{\partial h}{\partial \phi} \frac{\partial V}{\partial \phi} e^h + V e^h \frac{\partial^2 h}{\partial \phi^2} + V e^h \left(\frac{\partial h}{\partial \phi} \right)^2 \quad (F.4)$$

Substituting (F.4) into (F.1) yields

$$\begin{aligned} \frac{\partial V}{\partial r} = & \phi \frac{\partial^2 V}{\partial \phi^2} + \frac{\partial V}{\partial \phi} \left[2\phi \frac{\partial h}{\partial \phi} + 1 + c\phi \right] \\ & + V \left[\phi \frac{\partial^2 h}{\partial \phi^2} + \phi \left(\frac{\partial h}{\partial \phi} \right)^2 + \frac{\partial h}{\partial \phi} + c\phi \frac{\partial h}{\partial \phi} - \frac{\partial h}{\partial r} \right] \end{aligned} \quad (F.5)$$

Now suppose

(i) the coefficient of V in (F.5) is equal to $A + B\phi$ where A and B are constants

and

(ii) $(2\phi \frac{\partial h}{\partial \phi} + c\phi)$ in the coefficient of $\partial V / \partial \phi$ is equal to $2b\phi$ where b is a constant

Then Equation (F.5) becomes

$$\frac{\partial V}{\partial \tau} = \phi \frac{\partial^2 V}{\partial \phi^2} + (1 + 2b\phi) \frac{\partial V}{\partial \phi} + (A + B\phi)V \quad (\text{F.6})$$

From supposition (ii),

$$2\frac{\partial h}{\partial \phi} + C(\tau) = 2b \quad (\text{F.7})$$

which implies that

$$h = (b - \frac{C(\tau)}{2})\phi + f(\tau) \quad (\text{F.8})$$

where $f(\tau)$ is an arbitrary function of τ . Furthermore, it can be shown that

$$\frac{\partial^2 h}{\partial \phi^2} = 0 \quad (\text{F.9})$$

and

$$\frac{\partial h}{\partial \tau} = \frac{df(\tau)}{d\tau} - \frac{\phi}{2} \frac{dC(\tau)}{d\tau} \quad (\text{F.10})$$

Supposition (i) gives

$$\phi \frac{\partial^2 h}{\partial \phi^2} + \phi \left(\frac{\partial h}{\partial \phi} \right)^2 + \frac{\partial h}{\partial \phi} + C\phi \frac{\partial h}{\partial \phi} - \frac{\partial h}{\partial \tau} = A + B\phi \quad (\text{F.11})$$

Substituting (F.7), (F.8), (F.9) and (F.10) into (F.11), rearranging and equating coefficients of ϕ and the constant terms give

$$A = b - \frac{C}{2} - \frac{df(\tau)}{d\tau} \quad (\text{F.12})$$

and

$$B = b^2 - \left(\frac{C}{2}\right)^2 + \frac{1}{2} \frac{dC(\tau)}{d\tau} \quad (\text{F.13})$$

From (F.12),

$$f(\tau) = (b-A)\tau - \int_0^\tau \frac{C}{2} d\tau \quad (\text{F.14})$$

Substituting into (F.8) gives

$$h(\tau) = \left(b - \frac{C}{2}\right)\tau + (b-A)\tau - \int_0^\tau \frac{C}{2} d\tau \quad (\text{F.15})$$

Note that C is restricted by (F.13) where

$$\frac{dC}{d\tau} = 2(B-b^2) + \frac{C^2}{2} \quad (\text{F.16})$$

It can be shown readily that

$$C(\tau) = -k \tanh\left(\frac{k\tau}{2}\right) \quad (\text{F.17})$$

where

$$k = 2(b^2 - B)^{1/2} \quad (\text{F.18})$$

Therefore $C(\tau)$ is restricted to the functional form of (F.17) where k is an arbitrary constant.

Combining (F.3) and (F.15) gives

$$T = Ve^h = Ve^{(b-C/2)\phi} \exp\left((b-A)\tau - \int_0^\tau \frac{C}{2} dx\right) \quad (F.19)$$

By setting b and A to zero, (F.19) becomes

$$T = V \exp\left(-\frac{C}{2}\phi\right) \exp\left(-\int_0^\tau \frac{C}{2} dx\right) \quad (F.20)$$

Equation (F.6) becomes

$$\frac{\partial V}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + \frac{\partial V}{\partial \phi} + B\phi V \quad (F.21)$$

Rewriting (F.21) in terms of k gives

$$\frac{\partial V}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + \frac{\partial V}{\partial \phi} - \frac{k^2}{4} \phi V \quad (F.22)$$

Which is a differential equation with time invariant coefficients. Here C is not exact but is approximated by (F.17) with k being arbitrary. The transformation from T to V is given by (F.20) which can be further simplified as illustrated below.

$$\text{With } C = -k \tanh\left(\frac{kx}{2}\right),$$

$$\int_0^\tau \frac{C}{2} dx = \int_0^\tau \frac{-k \tanh(kx/2)}{2} dx$$

$$= -\log \left(\cosh \left(\frac{k\tau}{2} \right) \right)$$

Therefore,

$$\begin{aligned} \exp \left(- \int_0^\tau \frac{C}{2} dx \right) &= \exp \left(\log \left(\cosh \left(\frac{k\tau}{2} \right) \right) \right) \\ &= \cosh \left(\frac{k\tau}{2} \right) \end{aligned} \quad (F.23)$$

Equation (F.20) then becomes

$$T = V \cosh \left(\frac{k\tau}{2} \right) \exp \left(\frac{k\phi}{2} \tanh \left(\frac{k\tau}{2} \right) \right) \quad (F.24)$$

Finally, it can be shown that the initial and boundary conditions of (F.2) become

$$(i) \text{ at } \tau = 0, V = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial V}{\partial \tau} = \frac{\partial V}{\partial \phi}$$

$$(iii) \text{ at } \phi = \phi_0, \frac{\partial V}{\partial \phi} = \frac{C}{2} V \quad (F.25)$$

$$+ q(\tau) \operatorname{sech} \left(\frac{k\tau}{2} \right) \exp \left(\frac{-k\phi_0}{2} \tanh \left(\frac{k\tau}{2} \right) \right)$$

For the temperature boundary condition case where $T = g(\tau)$ at $\phi = \phi_0$, Equation (iii) of (F.25) is replaced by $V = g(\tau) \operatorname{sech}(k\tau/2) \exp(-k\phi_0/2 \tanh(k\tau/2))$.

APPENDIX G

SERIES SOLUTIONS FOR THE UNCOUPLED LIQUID-PHASE THERMAL DIFFUSION EQUATION WITH TIME VARYING C

It was shown in the Appendix F that with the following change of variables:

$$V(\tau, \phi) = T(\tau, \phi) \operatorname{sech}(k\tau/2) \exp((-k\phi/2) \tanh(k\tau/2)) \quad (\text{G.1})$$

the following equation

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + [1 + C(\tau)\phi] \frac{\partial T}{\partial \phi} ; 0 \leq \phi \leq \phi_0 \quad (\text{G.2})$$

and the associated initial and boundary conditions

$$(i) \quad \text{at } \tau = 0, T = 0$$

$$(ii) \quad \text{at } \phi = 0, \frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$$

$$(iiia) \quad \text{at } \phi = \phi_0, \frac{\partial T}{\partial \phi} = q(\tau) \quad (\text{G.3})$$

or

$$(iiib) \quad \text{at } \phi = \phi_0, T = g(\tau)$$

can be transformed to

$$\frac{\partial V}{\partial \tau} = \frac{\partial^2 V}{\partial \phi^2} + \frac{\partial V}{\partial \phi} - \frac{k^2}{4} \phi V ; 0 \leq \phi \leq \phi_0 \quad (\text{G.4})$$

and

$$(i) \text{ at } \tau = 0, V = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial V}{\partial \phi} = \frac{\partial V}{\partial \tau}$$

$$(iiia) \text{ at } \phi = \phi_0, \frac{\partial V}{\partial \phi} = \frac{C}{2} V + q(\tau) \operatorname{sech}(k\tau/2) \exp(C\phi_0/2) \quad (G.5)$$

$$(iiib) \text{ at } \phi = \phi_0, V = g(\tau) \operatorname{sech}(k\tau/2) \exp(C\phi_0/2)$$

where $C(\tau)$ as approximated by

$$C = -k \tanh(k\tau/2)$$

and the constant k is determine such that it will provide the best fit to a given function c .

In the boundary conditions above, (iiia) represents the temperature gradient boundary condition case and (iiib) corresponds to the temperature boundary condition case. The solutions for both cases are presented in this appendix.

Temperature Boundary Condition

Consider the following equation

$$\frac{\partial w}{\partial \tau} = \phi \frac{\partial^2 w}{\partial \phi^2} + \frac{\partial w}{\partial \phi} - \frac{k^2}{4} \phi w ; 0 \leq \phi \leq \phi_0 \quad (G.6)$$

together with the initial and boundary conditions given by

$$(i) \text{ at } \tau = 0, w = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial w}{\partial \tau} = \frac{\partial w}{\partial \phi}$$

$$(iii) \text{ at } \phi = \phi_0, w = 1 \quad (G.7)$$

The solution for w can be used to obtain solution for V by means of superposition.

Taking the Laplace Transform of Equations (G.6) and (G.7) on τ gives

$$\phi \frac{d^2 w}{d\phi^2} + \frac{dw}{d\phi} - \left(\frac{k^2}{4}\phi + S\right)w = 0 \quad (G.8)$$

and

$$(i) \text{ at } \phi = 0, Sw(S, 0) = \frac{dw}{d\phi}(S, 0)$$

$$(ii) \text{ at } \phi = \phi_0, w(S, \phi_0) = \frac{1}{S} \quad (G.9)$$

where A is the variable in the Laplace Transform.

Since $\phi = 0$ is a regular singular point in Equation (G.8), the method of Frobenius is used to obtain the series solutions. Assuming a series solution of the form

$$w = \sum_{n=0}^{\infty} A_n \phi^{n+a} \quad (G.10)$$

with the exponent a and all the coefficients A_n still undetermined. By differentiating twice, we have

$$\frac{dw}{d\phi} = \sum_{n=0}^{\infty} (n+a) A_n \phi^{(n+a-1)} \quad (\text{G.11})$$

and

$$\frac{d^2w}{d\phi^2} = \sum_{n=0}^{\infty} (n+a)(n+a-1) A_n \phi^{(n+a-2)} \quad (\text{G.12})$$

Substituting Equations (G.10), (G.11), and (G.12) into Equation (G.8) gives

$$\begin{aligned} & \sum_{n=0}^{\infty} (n+a)(n+a-1) A_n \phi^{(n+a-1)} + \sum_{n=0}^{\infty} (n+a) A_n \phi^{(n+a-1)} \\ & - \sum_{n=0}^{\infty} s A_n \phi^{(n+a)} - \sum_{n=0}^{\infty} \frac{k^2}{4} A_n \phi^{(n+a+1)} = 0 \end{aligned} \quad (\text{G.13})$$

After rearranging terms, it becomes

$$\begin{aligned} & a^2 A_0 \phi^{(a-1)} + ((a+1)^2 A_1 - s A_0) \phi^a \\ & + \sum_{n=0}^{\infty} \left[(n+a+2)^2 A_{n+2} - s A_{n+1} - \frac{k^2}{4} A_n \right] \phi^{(n+a+1)} = 0 \end{aligned} \quad (\text{G.14})$$

The uniqueness of power series requires that the coefficients of each power of ϕ on the left-hand side of Equation (G.14) must vanish individually. The requirement that the coefficient of $\phi^{(a-1)}$ vanishes yields

$$a^2 A_0 = 0 \quad (\text{G.15})$$

Since A_0 had been chosen as the coefficient of the lowest nonvanishing term of the series, Equation (G.10), hence, by definition, $A_0 \neq 0$. Therefore, we have

$$a^2 = 0 \quad (G.16)$$

which implies that $a = 0$

The requirement that the coefficient of ϕ^a vanish gives

$$A_1 = SA_0 \quad (G.17)$$

The requirement that the coefficient of $\phi^{(n+2)}$, ($n \geq 0$), vanishes gives

$$A_{n+2} = \frac{SA_{n+1} + (k^2/4) A_n}{(n+2)^2} \quad (G.18)$$

which is a three-term recurrence relation. Given A_0 and A_1 , A_2 can be computed and then A_3 , A_4 , and so on up as far as desired. Here since the two roots of the individual equation (i.e. Equation G.16) are equal, only one series solution can be obtained by the present method. The other independent series solution of w will be singular at $\phi = 0$ and since w is finite there, no attempt is made to seek that second independent solution.

Hence,

$$w(S, \phi) = A_0 W(S, k, \phi) \quad (G.19)$$

where, for brevity,

$$W(S, k, \phi) = 1 + \sum_{n=0}^{\infty} \left(\frac{A_n}{A_0} \right) \phi^n \quad (G.20)$$

Substituting (G.19) into (ii) of (G.9) gives

$$A_0 = \frac{1}{SW(S, k, \phi_0)} \quad (G.21)$$

Therefore,

$$w(\phi, S) = \frac{W(S, k, \phi)}{SW(S, k, \phi_0)} \quad (G.22)$$

It can be verified easily that (i) of (G.9) is satisfied by Equation (G.19) also.

By the Inversion Integral Technique,

$$w(\phi, \tau) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{S\tau} W(S, k, \phi)}{SW(S, k, \phi_0)} dS \quad (G.23)$$

Now $W(S, k, \phi_0)$ has simple zeros, S_n , where $W(S_n, k, \phi_0) = 0$. Thus the integrand has simple poles at $S = S_n$ and also at $S = 0$. By using the method of residues, we have:

Residue, R_0 , of integrand at $S = 0$:

$$\begin{aligned} R_0 &= \lim_{S \rightarrow 0} \frac{e^{S\tau} W(S, k, \phi)}{W(S, k, \phi_0)} \\ &= \frac{W(0, k, \phi)}{W(0, k, \phi_0)} \end{aligned} \quad (G.24)$$

Residue, R_n , of integrand at $S = S_n$:

$$R_n = \lim_{S \rightarrow S_n} \frac{(S - S_n) e^{S\tau} W(S, k, \phi)}{SW(S, k, \phi_0)} \quad (G.25)$$

$$\begin{aligned}
&= \lim_{S \rightarrow S_n} \frac{(S - S_n)}{W(S, k, \phi_0)} \cdot \lim_{S \rightarrow S_n} \frac{e^{S\tau} W(S, k, \phi)}{S} \\
&= \frac{e^{S_n \tau} W(S_n, k, \phi)}{S_n W_S(S_n, k, \phi_0)}
\end{aligned} \tag{G.26}$$

where L' Hospital rule has been used in obtaining the first limit and W_S denotes partial derivative of W with respect to S . Then

$$\begin{aligned}
w(\tau, \phi) &= \sum_{n=0}^{\infty} R_n \\
&= \frac{W(0, k, \phi_0)}{W(0, k, \phi_0)} + \sum_{n=1}^{\infty} \frac{W(S_n, k, \phi) e^{S_n \tau}}{S_n W_S(S_n, k, \phi_0)}
\end{aligned} \tag{G.27}$$

By means of Duhamel's Integral Technique,

$$V(\tau, \phi) = w(\tau, \phi)g(0) + \int_0^\tau w(\tau-x, \phi) \frac{dh(x)}{dx} dx \tag{G.28}$$

where

$$h(\tau) = g(\tau) \operatorname{sech}(k\tau/2) \exp(-k\phi_0/2) \tanh(k\tau/2) \tag{G.29}$$

Temperature gradient boundary condition

Consider the following equation

$$\frac{\partial u}{\partial \tau} = \phi \frac{\partial^2 u}{\partial \tau^2} + \frac{\partial u}{\partial \phi} - \frac{k^2}{4} \phi u; \quad 0 \leq \phi \leq \phi_0 \tag{G.30}$$

together with the following initial and boundary conditions

$$(i) \text{ at } \tau = 0, u = 0$$

$$(ii) \text{ at } \phi = 0, \frac{\partial u}{\partial \tau} = \frac{\partial u}{\partial \phi}$$

and

$$(iii) \text{ at } \phi = \phi_0, \frac{\partial u}{\partial \phi} = 1 \quad (G.31)$$

As in the temperature boundary condition case, the solution for u can be used as a Green's function for obtaining V by means of superposition.

Taking the Laplace Transform of Equations (G.30) and (G.31) on τ gives

$$\phi \frac{d^2 u}{d\phi^2} + \frac{du}{d\phi} - \left(\frac{k^2}{4} \phi + S \right) u = 0 \quad (G.32)$$

and

$$(i) \text{ at } \phi = 0, Su(S, 0) = \frac{du}{d\phi}(S, 0)$$

$$(ii) \text{ at } \phi = \phi_0, \frac{du}{d\phi}(S, \phi_0) = \frac{1}{S} \quad (G.33)$$

Since Equation (G.32) is identical to Equation (G.8), the solution u is given by

$$u = A_0 W(S, k, \phi) \quad (G.34)$$

Substituting (G.34) into (ii) (G.33) gives

$$A_o = \frac{1}{SW_{\phi}(S, k, \phi_o)} \quad (G.35)$$

where subscript ϕ denotes partial derivative with respect to ϕ . Therefore,

$$u(S, \phi) = \frac{W(S, k, \phi)}{SW_{\phi}(S, k, \phi_o)} \quad (G.36)$$

By the Inversion Integral Technique,

$$u(\tau, \phi) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{S\tau} W(S, k, \phi)}{SW_{\phi}(S, k, \phi_o)} dS \quad (G.37)$$

Now $W_{\phi}(S, k, \phi_o)$ has simple zeros, S_n , where $W_{\phi}(S_n, k, \phi_o) = 0$. Thus the integrand has simple poles at $S = S_n$ and also at $s = 0$. By using the method of residues, we have:

Residue, R_o , of integrand at $S = 0$:

$$\begin{aligned} R_o &= \lim_{S \rightarrow S_n} \frac{e^{S\tau} W(S, k, \phi)}{SW_{\phi}(S, k, \phi_o)} \\ &= \frac{W(0, k, \phi)}{W_{\phi}(0, k, \phi_o)} \end{aligned} \quad (G.38)$$

Residue, R_n , of integrand at $S = S_n$:

$$\begin{aligned} R_n &= \lim_{S \rightarrow S_n} \frac{(S - S_n) e^{S\tau} W(S, k, \phi)}{SW_{\phi}(S, k, \phi_o)} \\ &= \lim_{S \rightarrow S_n} \frac{(S - S_n)}{W_{\phi}(S, k, \phi_o)} \lim_{S \rightarrow S_n} \frac{e^{S\tau} W(S, k, \phi)}{S} \end{aligned} \quad (G.39)$$

$$= \frac{e^{S_n \tau} W(S_n, k, \phi)}{S_n W_{\phi S}(S_n, k, \phi_0)} \quad (G.40)$$

where L' Hospital rule has again been used in obtaining the first limit and $W_{\phi S}$ denotes the partial derivative of W with ϕ and S . Then

$$\begin{aligned} u(\tau, \phi) &= \sum_{n=0}^{\infty} R_n \\ &= \frac{W(0, k, \phi)}{W_{\phi}(0, k, \phi_0)} + \sum_{n=0}^{\infty} \frac{e^{S_n \tau} W(S_n, k, \phi)}{S_n W_{\phi S}(S_n, k, \phi_0)} \end{aligned} \quad (G.41)$$

By means of Duhamel's Integral Technique,

$$V(\tau, \phi) = u(0, \phi)h(0) + \int_0^{\tau} u(\phi, \tau-x) \frac{dh(x)}{dx} dx \quad (G.42)$$

where

$$h(\tau) = \frac{c}{2} F + q(\tau) \operatorname{sech}(k\tau/2) \exp(c\phi_0/2) \quad (G.43)$$

Substituting $h(\tau)$ into (G.42) gives

$$\begin{aligned} V(\tau, \phi) &= u(0, \phi) \left[f(\tau) + \frac{1}{2} C(\tau) V(\tau, \phi_0) \right] \\ &\quad + \int_0^{\tau} \frac{\partial u(\tau-x, \phi)}{\partial \tau} f(x) dx \\ &\quad + \frac{1}{2} \int_0^{\tau} c(x) V(x, \phi_0) \frac{\partial u(\tau-x, \phi)}{\partial \tau} dx \end{aligned} \quad (G.44)$$

FIGURES

Figure 2.1: Flow regions outside and within a fuel droplet at high Reynolds number. (After [7])

Figure 3.1: Core temperature versus ϕ at various time instants.

Figure 3.2: Surface temperature distribution at various time instants.

Figure 3.3: Surface fuel vapor mass fraction distribution at various time instants.

Figure 3.4: Hill's vortex and orthogonal streamline coordinates used in Prakash and Sirignano's Model. (After [2])

Figure 3.5: g_1 and g_2 versus ϕ .

Figure 3.6: Temperature versus ϕ comparisons at various time instants with unity temperature gradient boundary condition and $c = 0$.

Figure 3.7: Temperature versus ϕ comparisons at various time instants with unity temperature boundary condition and $c = 0$.

Figure 3.8: Temperature versus ϕ comparisons at various time instants with unity temperature gradient boundary condition and $c = 0.828$.

Figure 3.9: Temperature versus ϕ comparisons at various time instants with unity temperature boundary condition and $c = -0.828$.

Figure 3.10: Negative coefficient c versus time comparisons.

Figure 3.11: Temperature versus ϕ comparisons at various time instants with unity temperature boundary condition and time varying c .

Figure 5.1: Surface temperature versus time comparisons at various gas temperatures.

Figure 5.2: Non-dimensional radius versus time comparisons at various gas temperatures.

Figure 5.3: Coefficient c versus time comparisons at various gas temperatures.

Figure 5.4: Surface temperature versus time comparisons at various gas temperatures.

Figure 5.5: Non-dimensional radius versus time comparisons at various gas temperatures.

Figure 5.6: Coefficient c versus time comparisons at various gas temperatures.

Figure 5.7: Surface and vortex center temperature variation.

FIG.8 SURFACE AND VORTEX CENTER TEMPERATURE VARIATION

Figure 5.8: Surface and vortex center temperature variation.

Figure 5.9: Surface temperature versus time comparisons.

Figure 5.10: Droplet diameter versus time comparisons.

Figure 5.11: Total gas-phase heat flux versus time comparisons.

Figure 5.12: Liquid-phase heat flux versus time comparisons.

Figure 5.13: Surface temperature versus time comparisons.

Figure 5.14: Droplet diameter versus time comparisons.

Figure 5.15: Total gas-phase heat flux versus time comparisons.

Figure 5.16: Liquid-phase heat flux versus time comparisons.

Figure 5.17: Surface temperature versus time comparisons.

Figure 5.18: Droplet diameter versus time comparisons.

Figure 5.19: Total gas-phase heat flux versus time comparisons.

Figure 5.20: Liquid-phase heat flux versus time comparisons.

Figure 5.21: Negative coefficient c versus time comparisons.

Figure 6.1: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.2: Surface temperature versus time comparisons.

Figure 6.3: Overall mass ratio versus time comparisons.

Figure 6.4: Surface gas-phase mass fraction of heptane versus time comparisons.

Figure 6.5: Surface gas-phase fuel mass fraction versus time comparisons.

Figure 6.6: Droplet diameter versus time comparisons.

Figure 6.7: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.8: Surface temperature versus time comparisons.

Figure 6.9: Overall mass ratio versus time comparisons.

Figure 6.10: Surface gas-phase mass fraction of heptane versus time comparisons.

Figure 6.11: Surface gas-phase fuel mass fraction versus time comparisons.

Figure 6.12: Droplet diameter versus time comparisons.

Figure 6.13: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.14: Surface temperature versus time comparisons.

Figure 6.15: Overall mass ratio versus time comparisons.

Figure 6.16: Surface gas-phase mass fraction versus time comparisons.

Figure 6.17: Surface gas-phase fuel mass fraction versus time comparisons.

Figure 6.18: Droplet diameter versus time comparisons.

Figure 6.19: Surface temperature versus time comparisons.

Figure 6.20: Surface gas-phase fuel mass fraction versus time comparisons.

Figure 6.21: Droplet diameter versus time comparisons.

Figure 6.22: Surface temperature versus time comparisons.

Figure 6.23: Droplet diameter versus time comparisons.

Figure 6.24: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.25: Relative vaporization mass flux of hexane versus time comparisons.

Figure 6.26: Total vaporization mass flux versus time comparisons.

Figure 6.27: Total gas-phase heat flux versus time comparisons.

Figure 6.28: Liquid-phase heat flux versus time comparisons.

Figure 6.29: Surface temperature versus time comparisons.

Figure 6.30: Droplet diameter versus time comparisons.

Figure 6.31: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.32: Relative vaporization mass flux of hexane versus time comparisons.

Figure 6.33: Total vaporization mass flux versus time comparisons.

Figure 6.34: Total gas-phase heat flux versus time comparisons.

Figure 6.35: Liquid-phase heat flux versus time comparisons.

Figure 6.36: Surface temperature versus time comparisons.

Figure 6.37: Droplet diameter versus time comparisons.

Figure 6.38: Surface liquid-phase heptane mass fraction versus time comparisons.

Figure 6.39: Relative vaporization mass flux of hexane versus time comparisons.

Figure 6.40: Total vaporization mass flux versus time comparisons.

Figure 6.41: Total gas-phase heat flux versus time comparisons.

Figure 6.42: Liquid-phase heat flux versus time comparisons.

Figure 6.43: Negative coefficient c versus time comparisons.

Figure 6.44: Maximum percentage error in mass vaporization rate versus CPU time comparison.

Figure 8.1: Surface temperature versus time comparisons.

Figure 8.2: Non-dimensional radius square versus time comparisons.

Figure 8.3: Surface temperature versus time comparisons.

Figure 8.4: $(R/R_0)^{3/2}$ versus time comparisons.

Figure 8.5: Surface temperature versus time comparisons.

Figure 8.6: $(R/R_0)^{3/2}$ versus time comparisons.

Figure 8.7: Fuel vapor mass fraction versus distance at various times for different liquid-phase models.

Figure 8.8: Fuel vapor mass fraction versus distance at 16 milliseconds for different liquid-phase models.

Figure 8.9: Fuel vapor mass fraction versus distance at various times for the vortex model.

Figure 8.10: Gas-phase temperature versus distance at 16 milliseconds for different liquid-phase models.

Figure 8.11: Fuel vapor mass fraction versus distance at 16 milliseconds for different gas-phase models.

Figure 8.12: Gas-phase temperature versus distance at 16 milliseconds for different liquid-phase models.

Figure 9.1: Overall view of experiment. (After [27])

Figure 9.2: Air velocity and temperature versus distance downstream.
(After [27])

Figure 9.3: Distance downstream versus time. (After [27])

Figure 9.4: Droplet composition Versus distance downstream. (After [27])

Figure 9.5: Droplet diameter versus distance downstream. (After [27])

Figure 9.6: Air velocity and temperature versus distance downstream.
(After [27])

Figure 9.7: Distance downstream versus time. (After [27])

Figure 9.8: Droplet composition versus distance downstream. (After [27])

Figure 9.9: Droplet diameter versus distance downstream. (After [27])

Figure A.1: Surface temperature versus time comparisons

VOL. II. FUEL DROPLET VAPORIZATION EXPERIMENT

Abstract

Experimental results are presented for single and bicomponent droplets vaporizing in a hot, convective environment. Droplet sizes ranged from 160 to 360 microns and Reynolds numbers ranged roughly from 10 to 200. The experiments employ a free droplet technique whereby droplets are allowed to move freely in the experimental environment.

A generalized analysis of heat and mass transfer from vaporizing droplets is presented. A method is outlined by which the new data may be compared with the predictions of various vaporization models. Results show that the change of droplet composition is sensitive to the liquid phase model assumed, and support the existence of the vortex model described in Volume I. A gas phase model which compared well with previously obtained data is shown to overpredict droplet vaporization rates at lower Reynolds numbers, and a new gas phase model is presented which offers significant improvements. Some limitations of the film property approach in accounting for variable property effects are discussed.

Introduction

Vaporization of droplets plays a central role in many engineering systems. Notable examples include spray drying and the combustion of sprays. Although in many cases droplets exist in ensembles in which mutual interactions can introduce substantial complexities, an understanding of individual droplet vaporization behaviour is necessary to provide the foundation from which to approach these complexities. Thus, the study of individual droplet vaporization remains of interest and finds wide application.

In predicting droplet heat and mass transfer rates, many semi-empirical correlations have been derived from data obtained while holding droplets stationary during vaporization by some external means [1-6]. In this "stationary droplet" approach, the droplet is immobilized by hanging it from a fibre or thermocouple, or else the drop is simulated as a porous sphere whose surface is kept saturated with liquid supplied at a constant rate through a support structure. Experiments of this type offer superior control and ease of measurement, but they all suffer the common drawback that the support structure itself can significantly affect the quantities being measured. Liquid phase processes are in particular greatly perturbed, so the method can really be used to study steady state gas phase processes only.

More realistic but more difficult to perform are free droplet experiments in which the droplets remain free to move about in the experimental environment. Although there have been a number of these experiments (see the reviews by Williams[7], and Law[8]), relatively few of these have been directed towards studying the vaporization of isolated droplets, and few involve droplet Reynolds numbers greater than 10 or so. For example, in measuring vaporization and/or burning rates of droplets of various fuels falling freely through a furnace, Eisenklam, et al.[9], in a typical experiment, seldom obtained Reynolds numbers greater than 20, and mostly in the range less than 10. There are some exceptions. Miura, et al.[10] obtained Reynolds numbers in the range 980-1620 by floating 3mm water droplets in an upward flowing stream of air. Another exception is Lerner, et. al. [11,12], whose experiment will presently be discussed at length.

Aside from recent work done in connection with droplet microexplosion phenomenon, few workers have chosen to perform controlled experiments on non-exploding droplets containing more than one miscible component. Yet most practical fuels are neither chemically pure nor do they undergo microexplosions to any considerable extent. Furthermore, extensive theoretical work [13,14, and Vol. I] has shown that the liquid phase of such droplets tends to remain unsteady during much of the droplet lifetime. The manner of this unsteadiness provides the coupling necessary to establish gas phase behaviour, and has not been fully established experimentally. As discussed earlier, such information would need to be established using free droplet experiments.

It may be concluded, therefore, that there exists a need to conduct free droplet experiments of pure and multicomponent droplets in the range of droplet Reynolds numbers greater than about 10. Such experiments would provide information concerning liquid phase transient behaviour as well as provide confirmation of the gas phase results provided by previous stationary droplet experiments.

One such experiment has been devised by Lerner[12]. In that experiment, freely flowing single and bicomponent droplets have been studied roughly in the range $100 < Re < 200$. This Reynolds number range is of practical interest when vaporization occurs at higher pressures, such as in internal combustion engines. The results of this experiment have already been discussed in [11-12] and in Vol. I, so nothing further will be said about them here.

The objective of the present work has been to extend the range of Lerner's free droplet experiments. Attention has focused on single and bicomponent droplet vaporization in the range $10 < Re < 100$, which is of interest when vaporization occurs near atmospheric pressure, such as in spray drying or in oil burners. Some efforts were also made to obtain data in the range $100 < Re < 200$ but at higher vaporization rates than those of Lerner.

In the next section, the experimental apparatus is described. Following that, results are presented and discussed.

Experimental Apparatus

The experimental apparatus is the basic device used by Lerner and has been fully described in [12]. What follows is a brief summary.

An overall view of the experiment is given in Fig. 1. Heated air enters the bottom of the experiment, where a chamber allows the air to distribute more or less uniformly before the air rises to encounter several layers of stainless steel ball bearings. The ball bearings, a honeycomb, screens, a settling area, and a converging nozzle then provide thermal stability, flow straightening, and turbulence reduction. The air exits the converging nozzle as a laminar flow and passes through a 75cm long, 3.8cm I.D. pyrex test section having three flats along its length to provide optical access. The flow velocity in the test section is limited to about 25m/sec. Above this velocity, turbulence in the air stream reaches unacceptable levels.

At the base of the test section, droplets are injected into the air stream at low velocity with known frequency, entrained by the flowing air, and carried upwards into the test section where they vaporize. The droplet generator, shown in Fig. 2, relies on a piezoelectric principle. Two piezoelectric crystals are attached on either side of a slightly flattened stainless steel tube. Upon receipt of an electric pulse, the strips flex inwards to eject a drop from the glass orifice. To provide indication of fuel temperature prior to ejection, a thermocouple is mounted close to the tip of the orifice. Pulses are delivered to the generator at a frequency low enough so that the droplets do not exhibit mutual interference effects in the test section. The generator is capable of generating droplets ranging in diameter from 50-500 μ m.

The fuels used in this experiment were n-heptane and n-dodecane. They were chosen because their volatilities are significantly different and because their properties are well documented. The fuel is kept from boiling in the experiment by surrounding the droplet generator and supply piping with a water-fed cooling jacket. Because the tip of the generator is only about one square millimeter in area, there is no way, beyond a certain temperature, to provide adequate cooling to the tip without making major design changes. For heptane, boiling in the tip limited the maximum average test section temperature to somewhere around 675 deg. K.

A microscope/camera arrangement, shown in Fig. 3, mounted on a movable optical table provides the ability to measure droplet diameters at various positions in the test section. When a droplet passes both through the laser beam and the focus of the iris and lens system, reflected light from the droplet causes the photo multiplier tube to trigger the flash. A photograph is taken by leaving the camera shutter open while the room is darkened until a flash occurs.

Droplet composition is measured by collecting the droplets with a water-cooled probe which is inserted through the ball valve at the top of the test section. Two probes are used to collect droplets at different rates. The probe shown in Fig. 4. The smaller probe is made from pyrex while the larger one is made

from quartz to reduce thermal stress.

A schematic of the probe is shown in Fig. 5. The central portion of the probe is an orifice open to the surroundings which is filled part way with a column of water. When the probe is inverted, open end down, and inserted through the ball valve into the droplet laden air stream, the column remains stable due to surface tension at the meniscus. Droplets striking the meniscus penetrate through and collect at the top of the orifice, where further vaporization is prohibited. An absorbant cloth lines the leading inside portions of the orifice. The cloth acts as a wick to draw off and vaporize the liquid fuel which does not penetrate the meniscus. When a sufficient number of droplets have been collected, the probe is withdrawn and the sample removed from the orifice with a hypodermic syringe. The sample is then injected into a gas chromatograph for analysis.

It has been discovered that below a certain size and velocity, droplets no longer penetrate the meniscus. Below some threshold kinetic energy, the droplets either bounced off or remained at the interface to eventually vaporize. Addition of surfactants to the water in the orifice helped somewhat, but generally the probe was not usable in the Reynolds number range $10 < Re < 100$ which was being investigated. Composition measurements were therefore not performed in this Reynolds number range. Instead, for multicomponent data taken in this range, the initial composition was estimated from knowledge of the composition in the fuel reservoir.

Measurement of the droplet velocity was performed using a stroboscopic technique. By setting the strobe period slightly longer than the droplet period, the droplets could be made to appear to slowly rise in the test section. The time required for the droplets to rise to various positions in the test section was then converted to the real time required for a single droplet to reach those positions by multiplying by a constant factor which depends on the strobe and droplet periods.

Air velocities in the test section are measured by extending a linear rake of five pitot tubes to various positions in the test section. At each position the probes are oriented across the test section as shown in Fig. 6. Air temperatures are obtained by extending a similar rake of five thermocouple probes.

Smoke tests have confirmed a small but finite level of turbulence in the test section. Because of this, droplets do not always follow exactly the same path through the test section. This accounts for the fact that when the stroboscopic technique is used to measure droplet velocities, the droplets appear frozen as droplet clusters rather than as individual droplets, because the strobe does not stop each droplet at exactly the same position. Accordingly, when interpreting the air temperature and air velocity profiles, it is useful to have some means of determining the temperature and velocity histories which an average droplet undergoes. The method used in [12], though not the only possible method, is a plausible one and has been adopted here also. It goes as follows. The width of the droplet clusters

as observed with the stroboscope tends to grow approximately linearly with distance. Measurement of the width of these clusters at various heights yields a linear least square fit of cluster radius r vs. distance. At a given distance, temperatures and velocities at widths $r/2$ and r , on both sides of the center, are determined using a linear interpolation of probe readings, while values at the center are known from the probe at position 3. A center weighted average of these five values is then computed by weighting the center value by a factor of 6, the values at $r/2$ by a factor of 2, and the values at r by a factor of one. Finally, a third order least square fit of the center weighted averages at different heights is computed.

Presentation of Data

Experimental data has been obtained in five separate runs and is presented in detail in Figures 7-29. A summary of experimental conditions is given in Table 1. Only one experiment, Run 1, was performed under the higher convective conditions of approximately $100 < Re < 200$. The other experiments were performed where roughly $Re < 100$. In Run 2, pure n-heptane drops were used, and in Runs 3-5, droplets contained a mixture of n-heptane and n-dodecane. Because Reynolds numbers are a strong function of the film property rules used to evaluate them, explicit Reynolds number ranges are intentionally not given.

In his work, Lerner[12] measured the degree to which droplets are distorted from a spherical shape by the velocity field, and found that droplet distortion was small enough as to have a negligible effect on droplet trajectory, composition, and vaporization rates. Although the validity of these conclusions is not examined in the present study, measurements have been taken of the ratio of the horizontal (i.e., perpendicular to the flow) droplet diameter to the vertical diameter for Runs 1 and 2. In Run 1, for which Reynolds number and droplet diameters were similar to those used by Lerner, results showed a degree of distortion similar to that reported by him. The results for Run 2 showed almost no distortion, which is reasonable since convective conditions were less severe and the droplets half as large. The results for Runs 3-5, not shown, are similar to those for Run 2.

A few remarks need to be made concerning the velocity and temperature profiles. The presence of the water-cooled bluff body creates a central core of relatively cooler, slower air in the test section down stream from it. This may be seen from the measurements by probes at position 3. Higher in the test section, the combined effects of mixing and boundary layer growth in the test section causes increasing temperatures and velocities at position 3, while those at the outer probe positions either fall or remain relatively constant depending on proximity to the wall. The growth of the boundary layer may be seen from the velocity measurements at positions 1 and 5. Runs 1 and 4, having higher velocities than the other runs, also exhibit a slight crosswise pressure gradient immediately downstream from the bluff body which causes a different rate of boundary layer growth on opposite sides of the test section. In Run 1, the pressure gradient has also caused a "washing" of hotter, faster air across the central areas of the test sections within 12 cm of the bluff body. Thus, the temperature and velocity at position 3 are seen to first dip slightly before rising.

Summary of Experimental
Conditions

Run No	Temp. range (K)	Velocity range (m/s)	Diameter range (μm)	$\frac{\text{Mass heptane}}{\text{Mass dodecane}}$
1	520-660	18-24	316-359	2.9
2	440-530	6-9	222-267	Pure n-heptane
3	485-550	7-9	190-210	0.5
4	520-680	14-21	188-208	0.5
5	395-460	6-8	163-182	0.4

Temperature and velocity ranges are for center weighted averages.

Table 1.

There is some qualitative difference in the profile shapes between Runs 1 and 2 and Runs 3-5. In Runs 3-5, the profiles are skewed towards higher temperatures and velocities at position 1, and at a given height tend to decrease as the test section is traversed horizontally. This is because the arrangement of ball bearings in the bottom of the experiment was different than shown in Fig. 1 for Runs 3-5. For those runs, the small mixing area below the ball bearings shown in Fig. 1 did not exist and was also filled with ball bearings. The air from the supply piping encountered the ball bearings immediately and was forced upwards by the flow resistance presented by the ball bearings. As a result, air tended to flow into the rest of the experimental apparatus only from the one quadrant of the ball bearings into which it was introduced by the air supply piping. This was confirmed by observing the pattern of discoloration of the ball bearings caused by the flow of hot air. The final result was that the velocity and temperature profiles in the test section were not symmetric and tended towards higher temperatures and velocities in the vicinity of probes 1 and 2, which are located in the same quadrant from which the air exited the ball bearings.

To correct this, some of the ball bearings were removed and the rest were elevated with a perforated plate and tripod support to a level higher than the entrance region. This is the configuration shown in Fig. 1. The space now provided below the ball bearings allows the air to spread more uniformly to all quadrants before encountering the resistance of the ball bearings. The resulting profiles, while not uniform, are more concentric, with higher temperatures and velocities tending to remain in the outer rings of the test section (until boundary layer growth). The resulting symmetry makes center weighted averaging more meaningful.

With the exception of the center weighted averages, curves shown on the temperature and velocity plots are not statistical fits. For the sake of clarity, they were drawn simply to connect the data points for a given probe position as a function of downstream distance. This, coupled with random measurement errors, "washing", and the manner of boundary layer growth, causes an appearance of irregularity on some of the profile plots. These irregularities are effectively smoothed by the center weighted averaging. Lerner[12] has found that the manner in which this average is taken did not strongly affect the theoretical comparisons he made.

Finally, it needs to be noted that the air velocity profile reported for Run 5 contains only the center weighted average and no other detailed velocity data. This is because it has been found from Runs 2, 3, and other trial runs not shown that when the air velocity is relatively low, such as in Run 5, the center weighted average so closely follows the velocity readings at position 3 that the difference is not significant. Since obtaining full velocity profiles takes quite a bit of time (6 hours), a great amount of time was saved by taking readings only at position 3. The center weighted average for Run 5 therefore represents a least square fit of the

velocity readings at position 3. Spot checking the readings of the other velocity probes confirmed the reasonableness of the measurements.

Generalized Analysis

Comparison of experimental data with the predictions of various models of droplet vaporization is the most important means by which both the data and the models are to be meaningfully evaluated. In the case of droplet vaporization, models which are currently available include semi-empirical correlations and other more fundamental theories such as those discussed in Volume I. Presented below is a generalized description of predictions made by droplet vaporization models with emphasis on predictions of overall heat and mass transfer rates. Following that, a method is outlined by which these predictions may be compared with the data generated by the present experiment.

The Nusselt and Sherwood numbers may be defined as

$$(1a) \quad Nu \equiv q_s'' / \left[k \frac{(T_\infty - T_s)}{D} \right]$$

$$(1b) \quad Sh \equiv m_s'' / \left[g D \frac{(Y_s - Y_\infty)}{D} \right].$$

The arrangement of symbols in (1) is intended to accent the nature of these numbers as normalized or non-dimensional heat and mass transfer rates. The heat and mass transfer predictions of any model may therefore be expressed in the form

$$(2) \quad Nu = Nu(Re, Pr, Bh)$$

$$(3) \quad Sh = Sh(Re, Sc, Bm)$$

These equations state that the dimensionless heat and mass transfer rates are functions of the Reynolds number, Prantl and Schmidt numbers, and mass transfer numbers which express the magnitude of the convective fluxes relative to the diffusive fluxes at the surface. For heat and mass fluxes, these numbers may be defined respectively as

$$(4) \quad Bh \equiv \frac{m_s'' c_p (T_\infty - T_s)}{-k \left(\frac{\partial T}{\partial r} \right)_s}$$

$$(5) \quad Bm \equiv \frac{m_s'' (Y_s - Y_\infty)}{-g D \left(\frac{\partial Y}{\partial r} \right)_s}$$

For droplets vaporizing in air, the mass flux has a convective component and a diffusive component given by Fick's law:

$$(6) \quad m_s'' = \gamma_s m_s'' - s \mathcal{D} \left(\frac{\partial \gamma}{\partial r} \right)_s$$

or,

$$(7) \quad m_s'' = \frac{-s \mathcal{D}}{(1 - \gamma_s)} \left(\frac{\partial \gamma}{\partial r} \right)_s$$

The energy flux to the droplet also has a convective and a diffusive component,

$$(8) \quad e_s'' = m_s'' c_p T_s - K \left(\frac{\partial T}{\partial r} \right)_s$$

However, unlike the mass flux for which both the convective and the diffusive components flow in the same direction (outwards), these components of the energy flux flow in different directions. In steady state, the diffusive, or inward, component of the energy flux is related to the total mass flux through the latent heat, according to the relationship

$$(9) \quad -K \left(\frac{\partial T}{\partial r} \right)_s \equiv \dot{q}_s'' = L_s m_s''$$

By using eqns. (1), (4), and (5), this relationship may be expressed in a non-dimensionalized form which relates the Nusselt and Sherwood numbers,

$$(10) \quad \frac{Nu}{Sh} = \frac{B_m}{B_h Le} (1 - \gamma_s)$$

where $Le = \alpha / \mathcal{D}$ is the Lewis number. The presence of the factor $(1 - \gamma_s)$ in (10) and in other expressions which relate the Nusselt and Sherwood numbers for droplet vaporization is a direct consequence of accounting for the convective component of the mass flux in eqn. (6). For low vaporization rates, when the diffusive component is dominant, this factor is essentially unity.

By using eqn. (9) in (4), and eqn. (7) in (5), the following more familiar alternate expressions for B_h and B_m are obtained:

$$(11) \quad B_h = \frac{c_p (T_\infty - T_s)}{L_s}$$

$$(12) \quad B_m = \frac{(y_s - y_\infty)}{(1 - y_s)}$$

The foregoing developments have assumed steady state. In reality, however, droplet vaporization is an unsteady process. In the gas phase, this usually presents little problem because gas phase processes are typically so fast that steady state profiles are developed or nearly developed before any other parameter can change significantly. The gas phase may therefore be considered to be quasi-steady. If the liquid phase is also in steady state or nearly so, then all of eqns. (1 - 12) are still applicable. Furthermore, because Nusselt and Sherwood numbers may be directly determined using any two of eqns. (2), (3), and (10), one is given some latitude in choosing which of these equations to use.

Many times, however, the liquid phase cannot be considered to be in steady state. This becomes the case when the droplet itself is heating up or if it is composed of several chemical components which diffuse outward and vaporize at different rates. In this case, the energy transferred to the droplet from the gas phase becomes divided between vaporization and liquid phase heat up. Equation (9) then becomes

$$(13) \quad \dot{q}_s'' = L_s \dot{m}_s'' + \dot{q}_l'',$$

where $\dot{q}_l''$ is the energy used to increase droplet temperature which does not immediately contribute to vaporization. Equation (13) can be made to assume the form of eqn. (9) by defining an effective latent heat of vaporization,

$$(14) \quad L_s' \equiv L_s + \frac{\dot{q}_l''}{\dot{m}_s''}$$

Because an unsteady liquid phase generates a third unknown, all three of eqns. (2),

(3), and (10) must be used to determine the Nusselt and Sherwood numbers. Recall that eqn. (10) remains valid even in the unsteady case because it was derived using the definition of B_h given in eqn. (4), which remains unchanged. If one wishes to use the alternate expression (11), however, the effective latent heat L'_s must be used instead of L_s . That is, one must use

$$(15) \quad B'_h = \frac{c_p(T_\infty - T_s)}{L'_s}$$

For the general case, the method of solution now proceeds roughly as follows. First, calculate B_m using eqn. (12) and Sh using eqn. (3). Next, assume a value for q_1'' and calculate L'_s using (1) and (14). calculate B'_h and Nu using (15) and (2), then check the result in eqn. (10). Iterate until (10) is satisfied.

Because of uncertainties in the mass diffusion coefficient $\mathcal{D}$, and in mass transfer measurements in general, experimental Sherwood number correlations of the form (3) tend to be less accurate than Nusselt number correlations, and frequently one desires to avoid using them. For steady state calculations, this poses no problem because, knowing the Nusselt number, one can solve for the Sherwood number using eqn. (10). For an unsteady liquid phase, eqn. (3) must be replaced with some other relationship.

One possible way of finding such a relationship is to perform detailed gas phase calculations according to some comprehensive model from which the Sherwood number may be obtained in lieu of an empirical relationship. Once such calculations are performed, however, enough information is in most cases available to directly calculate the Nusselt number also. Therefore this method should more properly be considered to be a fundamental approach rather than an empirical approach.

In the absence of detailed calculations, the method most often used is to assume certain results derived from quasi-steady spherically symmetric droplet vaporization. By applying energy and mass balances to spherical shells surrounding the droplets and assuming constant properties, one obtains the well known result[15]

$$(16) \quad \dot{m}_s'' = \frac{2g\alpha}{D} \ln(1+B_h) = \frac{2g\alpha}{D} \ln(1+B_m)$$

From this and previous definitions one can easily obtain

$$(17) \quad Nu = 2 \frac{\ln(1+B_h)}{B_h}$$

$$(18) \quad Sh = \frac{2}{(1-\gamma_s)} \frac{\ln(1+B_m)}{B_m}$$

The relationship between B_m and B_h may be found by inserting (17) and (18) into (10), giving

$$(19) \quad B_h = (1+B_m)^{1/L_e} - 1$$

Often in the droplet vaporization literature the Lewis number is assumed to be unity. In that case, (19) reduces simply to

$$(20) \quad B_h = B_m$$

When the liquid phase is unsteady, B_h should be replaced with B_h' in (17 - 20).

As a way to replace eqn. (3), eqn. (19) is often assumed to hold even in non-symmetric convective vaporization. For an unsteady liquid phase, B_m is calculated using (12), and then used to calculate both Nu and B_h using (2) and (19). Then Sh is found using (10).

This method suffers from the obvious weakness that convective droplet vaporization is not spherically symmetric, so eqn. (19) may not even be valid. Another important weakness not as obvious arises when the effects of variable properties are important.

Gas phase properties often can vary significantly with distance from the droplet, particularly for high ambient temperatures and high vaporization rates. Lerner[12], for example, found that Reynolds numbers could be made to vary by as much as a factor of 6 for the conditions he studied depending on where the properties were evaluated. A typical method for dealing with variable properties, especially in connection with empirical correlations, is to introduce the concept of film properties. A film property is a weighted average of properties at the surface conditions and at ambient conditions,

$$(21) \quad \phi_b = \phi_s + r(\phi_\infty - \phi_s)$$

where $0 < r < 1$ and ϕ is some property. The relationships (2) and (3) are then expressed in terms of non-dimensional numbers which have been evaluated at film conditions.

In order to avoid inconsistencies, extreme care must be taken in using (21). Suppose, for example, that the fuel mole fraction at the film condition, X_f , is evaluated using (21). Then the corresponding mass fraction is given by

$$(22) \quad Y_b = \frac{X_b M_b}{X_b M_b + X_{air} M_{air}}$$

Equation (22) is an identity required by the definitions of mass fraction, mole fraction, and conservation of mass. If, in addition, Y_f is calculated using eqn. (21), then a simple substitution will show that the result will in general be inconsistent with eqn. (22). The same inconsistency problems apply to other properties. If one calculates a property at the surface and at infinity, and then averages according to (21), the result will in general be different than if the property is calculated at the film temperature T_f and mole fraction X_f .

What is normally done therefore is to apply eqn. (21) only to temperature and either mass fraction or mole fraction. Other properties are then evaluated by first calculating the pure phase properties at the film temperature, and then calculating the mixture properties using appropriate mixture relationships at the film mole fraction and mass fraction. There are, however, no consistent rules for defining the film condition. For example, Hubbard, et. al. [16] recommend applying eqn. (21) to temperature and mass fraction with $r = 1/3$, while Renksizbulut and Yuen[6] find that averaging temperature and mole fraction with $r = 1/2$ fits their data best.

The property averaging rule (21) can cause other kinds of inconsistency problems. A dramatic example may be found by returning to eqn. (19), which it will be recalled was derived from a spherically symmetric vaporization model. Table 2. presents properties of mixtures of air and heptane vapor above a body of pure liquid n-heptane at steady state, evaluated using the film conditions of Renksizbulut and Yuen, given above. With the exception of the two most right hand columns, the values in this table are taken directly from Renksizbulut[17], which was the source work for [6]. In this table, $Y_\infty = 0$. Given in one column are values of B_m as defined by eqn. (12). Because it is a function only of Y_s , which is evaluated only at the surface, B_m should be independent of any film property averaging schemes. Given in another

column is B_m calculated from known values of $B_{h,f}$ using eqn. (19). Since both $B_{h,f}$ and Le,f depend on film properties, so apparently does B_m when calculated in this fashion. For this reason, it is written as $B_{m,f}$ in this row. The difference between B_m and $B_{m,f}$ is given in the last column. The error is shown to reach 80%.

The reason for the discrepancy is clear. Equation (19) was a derived result which assumed, among other things, constant properties. Its application in a variable property situation is unjustified. It should be noted here that, although eqn. (19) was derived from eqn. (10), this conclusion does not invalidate eqn. (10) for variable properties. Equation (10) is properly independent of any film property calculation scheme. It is only when the improperly derived results (17) and (18) are inserted into (10) do the inconsistencies arise.

By varying the value of r in eqn. (21), the error ΔB in table 2. can be made to range from negative at all temperatures to positive at all temperatures. Furthermore, no value of r which has been tried has resulted in a consistently low error or even a consistent magnitude and sign. These facts point strongly towards severe limitations in the film property approach. On the one hand, theoretical calculations need to accurately account for property variations, while the film property approach represented by eqn. (21) may not accurately account for these variations. On the other hand, although experimental investigations such as [6] do seem to show that the film property approach has some success in representing a large amount of data as long as strictly empirical correlations are used, rules for evaluating film properties have not yet been agreed upon.

Up to this point, quasi-steady gas phase modeling of droplet vaporization has been discussed which has accounted both for steady and non-steady state liquid phase. It has been shown that the case of an unsteady liquid phase is a more constraining case which in general requires the solution of three equations in three unknowns. A method has been described by which less accurate Sherwood number correlations can be replaced with derived results from quasi-steady, spherically symmetric droplet vaporization with constant properties, along with the problems inherent in applying those results for variable property cases. Before closing this section, a few general comments will be made concerning liquid phase modeling and multicomponent droplet vaporization.

Thermophysical Properties of Heptane Vapor/Air Mixtures
(from [17])

T_{∞} (C)	T_c (C)	Y_s	$R_{h,f}$	Le,f	$B_{m,f}$	B_m	ΔB
100	36	.28	.201	2.29	.520	.388	-.132
200	55	.49	.558	1.64	1.06	.961	-.099
300	66	.65	1.08	1.23	1.47	1.86	.390
400	75	.76	1.75	.978	1.69	3.17	1.48
500	83	.85	2.57	.820	1.84	5.67	3.83
600	90	.92	3.62	.699	1.92	11.5	9.58

Table 2.

The extension of the equations in this section to multicomponent droplet vaporization is for the most part straight forward. Mixture property rules are generally given for any number of components. Where the mass fraction or mole fraction appears in a manner not connected with the properties of mixtures, such as in calculating B_m , one simply replaces them with a sum over all fuel species.

One area in which some care must be taken, is in determining mass diffusion coefficients D . In general, these coefficients are different for each component, and in multicomponent systems, their calculation is extremely complicated. Furthermore, in many cases, even binary diffusion coefficients are not always well known. What is usually done is to assume that all species diffuse at equal rates determined by some average diffusion coefficient, but considerable uncertainty exists in how to determine this average and the issue remains unresolved.

The effect of the liquid phase has so far been discussed only as it pertains to the liquid phase heat up term q_l'' . Before proceeding further, let it be noted that q_l'' is not so directly dependent on the liquid phase as it is on the gas phase. Having appropriate relationships for Nusselt and Sherwood numbers in the forms given by eqns. (2) and (3), one can, together with eqn. (10), solve for q_l'' knowing only the droplet surface temperature and composition. One applies q_l'' therefore as a boundary condition for calculating the response of the liquid phase. This boundary condition is of the form

$$(23) \quad g_l'' = -k_l \left(\frac{\partial T_l}{\partial r} \right)_s$$

The relevant outputs from the liquid phase model required as boundary conditions for the gas phase model are the surface temperature and composition. These affect the gas phase not only through the T_s term in eqns. (1) and (11), but also through the vapor pressure at the droplet surface, which determines Y_s . Since phase change at the droplet surface is one of the fastest of all droplet processes, it is usually assumed that phase equilibrium exists and that, knowing surface temperature and composition, the vapor pressure may be calculated using the Clausius-Clapeyron equation or other empirical relationship.

The form of the liquid phase temperature gradient in (23) depends on the specific liquid phase model used. Because of the relative inaccessibility of the liquid phase to direct experimental probing, liquid phase models tend to be largely theoretical in nature. Their differences most often revolve around the degree and nature of internal motion occurring within the droplet.

The simplest of the liquid phase models assumes that circulation within the droplet is vigorous enough to completely mix the interior. Liquid phase temperatures are then considered to be everywhere the same, and the droplet is modelled as spatially uniform though temporally varying. In this case, q_l'' finds its expression in the liquid phase as the energy necessary to heat the entire droplet mass uniformly. Eqn (23) becomes

$$(24) \quad \dot{q}_l'' = \frac{\rho_l c_{p,l} D}{6} \frac{dT_l}{dt}.$$

Once q_l'' is known from the gas phase solution, one integrates eqn. (24) to obtain the liquid phase temperature.

If one is dealing with multicomponent droplets, the liquid phase mass fraction must also be specified. For a bi-component droplet undergoing complete mixing, the liquid phase mass fraction is given by

$$(25) \quad Y_{a,l} = \frac{m_a}{m_t}$$

By differentiating this expression and assuming equal gas phase diffusivities, it can be shown [12] that

$$(26) \quad \frac{dY_{a,l}}{dt} = \left[\frac{Y_{a,s}}{Y_s} - Y_{a,e} \right] \frac{\dot{m}_s''}{\rho_l D},$$

where $Y_{a,s}$ and Y_s are the mass fraction of species a and the mass fraction of all fuel species, respectively, evaluated in the gas phase at the droplet surface. Given $\dot{m}_s''$, the liquid phase surface mass fraction is found by integrating eqn (26).

In reality, of course, it is unreasonable to expect that the droplet interior is completely mixed. In Volume I, for example, it was shown theoretically that under certain conditions surface stresses on the droplet induce internal circulation in the form of a Hill's spherical vortex within the droplet. Even when the action of this vortex might be described as vigorous, temperature and concentration gradients normal to the stream surfaces of this vortex remain significant, and the droplet

interior may not be considered uniform. It may be expected, therefore, that an accurate description of droplet vaporization will require that a non-uniform droplet interior be adequately accounted for.

The simplest of the non-uniform liquid phase models assumes that there is no internal circulation within the droplet and furthermore that the liquid phase is spherically symmetric. Although these assumptions are also not very realistic, the model represents a physical limit of droplet behavior and is relatively easy to formulate and to compute with. When contrasted with complete internal mixing, the results of the two models may be expected to bracket real droplet behavior. In some cases, such as when vaporization rates are low, the relative differences between the two extreme models may be tolerably small, in which case one need not seek more detailed models.

To compute the droplet surface temperature, one needs to solve the spherically symmetric conduction equation

$$(27) \quad \frac{\partial T_e}{\partial t} = \frac{\alpha_e}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T_e}{\partial r} \right) ; \quad 0 \leq r \leq R(t)$$

with boundary conditions

$$(28) \quad T_e(r, 0) = T_{e,0}(r)$$

$$(29) \quad \frac{\partial T_e}{\partial r}(0, t) = 0$$

$$(30) \quad -\kappa_e \left(\frac{\partial T_e}{\partial r} \right) (R(t), t) = g_e''$$

The moving boundary at $r = R(t)$ introduces a small complication which may be resolved by a suitable transformation of coordinates. Details of this transformation, and other details concerning this method may be found in [18].

For bi-component droplets, the liquid phase surface mass fraction may be found by solving a similar set of equations for mass transfer:

$$(31) \quad \frac{\partial y_{a,e}}{\partial t} = \frac{D_{ae}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial y_{a,e}}{\partial r} \right) ; \quad 0 \leq r \leq R(t)$$

$$(32) \quad y_{a,l}(r,0) = y_{a,l,0}(r)$$

$$(33) \quad \frac{\partial y_{a,l}}{\partial r}(0,t) = 0$$

$$(34) \quad m_s'' y_{a,l}(R(t),t) - S_e \omega_l \frac{\partial y_{a,l}}{\partial r}(R(t),t) = m_{a,s}''$$

where $m_{a,s}''$ is the mass flux of species a at the droplet surface, and depends on the gas phase model used. For a spherically symmetric gas phase, for example,

$$(35) \quad \frac{y_{a,s}}{y_s} m_s'' = m_{a,s}''$$

For more accurate results, more realistic liquid phase models need to be employed. The model presented in Volume I solves for heat and mass diffusion within the droplet normal to the stream surfaces of a Hill's Vortex inside the droplet. When the gas phase Reynolds number is greater than about 100, the circulation in the vortex has been shown to be sufficiently fast that temperatures and concentrations are uniformized on the stream surfaces. The result of this is that diffusion inside the droplet now occurs within a geometry which is specified by the shape of the vortex. Formulation of the diffusion equations and boundary conditions are more complicated in this geometry. The boundary condition (23) remains intact, however, although its expression may be in terms of different coordinates. For further details concerning this model, the reader is referred to Volume I of this report.

Comparison with Experimental Data

In addition to generally having an unsteady liquid phase, the droplets measured in the present experiment are also subjected to time varying ambient temperatures and relative velocities. To deal with this, the gas phase is assumed to be quasi-steady and the relationships described in the previous section are converted into systems of ordinary differential equations in order to perform comparisons. What follows is a brief outline of the means by which this is done. Many additional details, as applied to specific gas phase and liquid phase models, may be found in [12].

At a given time t , a bicomponent droplet of diameter $D(t)$ having an average surface temperature $T_s(t)$ and mass fraction $Y_s(t)$ occupies a position $x(t)$ and moves with velocity $V(t)$. It experiences an air temperature $T_\infty(x)$ and absolute air velocity $V_\infty(x)$ determined from temperature and velocity data by fitting a 3rd order least square fit to the center weighted averages as described earlier. With this information, one can find m_s'' , q_s'' , and q_l'' using expressions for Nusselt number and Sherwood numbers appropriate to the particular model being employed. Assuming the droplets are spherical, one may then obtain, using m_s'' ,

$$(36) \quad \frac{dD}{dt} = - \frac{2 m_s''}{\rho_l}$$

An appropriate relationship for the drag coefficient gives

$$(37) \quad \frac{dV}{dt} = \frac{3g}{4D\rho_l} |V_\infty - V| (V_\infty - V) C_D - g$$

The rate of change of droplet position is given simply by

$$(38) \quad \frac{dx}{dt} = V$$

Once the derivatives (36-38) are known, the next step is to apply the values found for m_s'' and q_l'' as boundary conditions for the liquid phase model to determine the values of surface temperature and composition at the next time step, i.e., $T_s(t + \Delta t)$ and $Y_s(t + \Delta t)$. Then, knowing the derivatives (36-38), new values $D(t + \Delta t)$, $V(t + \Delta t)$, and $x(t + \Delta t)$ may be determined by using a suitable numerical integration scheme.

For all the results presented in this report, the integration scheme used was a fourth order Runge-Kutta method. Finding $V_{\infty}(x + \Delta x)$ and $T_{\infty}(x + \Delta x)$ completes the cycle, and the process is repeated to compute the next time step.

The initial and boundary conditions for the calculation are prescribed as follows. At time zero, values for $D(0)$, $Y_{\infty}(0)$, $V(0)$, and $x(0)$ are determined from experimental data. It is assumed that $Y_{\infty} = 0$. The initial droplet temperature is set equal to the wet bulb temperature appropriate for the ambient conditions at the initial position $X(0)$. This is considered to be a very good approximation because measurements by the thermocouple located near the tip of the droplet generator indicate that fuel temperature is very close to the wet bulb temperature. It is also reasonable in consideration of the low fuel flow rates there combined with the fact that near the tip, cooling of the fuel can not be very effectively provided. The wet bulb temperature is defined as that temperature for which the appropriate gas phase models give $q_1'' = 0$.

In comparing the present data with various models, attention has thus far focused mainly on semi-empirical correlations because of the ease of calculation which they offer. Planned but not yet performed are comparisons with the more fundamental theories presented in Volume I. Preliminary results of comparisons made to date are presented below.

The experimental data has been compared with a semi-empirical model developed in [12] to evaluate the data previously generated by this experiment. The model combines classical spherically symmetric vaporization theory with a convective correction from Ranz and Marshall [1] in the gas phase, coupled with a complete mixing model in the liquid phase. In addition, the gas phase model has also been coupled with a spherically symmetric diffusion model in the liquid phase.

The gas phase model expresses the droplet vaporization rate as

$$(39) \quad m_s'' = \frac{2K}{c_p D} \ln(1+B_m) \left[1.0 + 0.3 Re^{1/2} Pr^{1/3} \right]$$

In eqn. (39), B_m is defined as in eqn (12), and is assumed equal to B_h as defined by eqn (15). This equality allows solution for the liquid phase heat-up term q_1'' . The Lewis number is assumed to be unity. The drag coefficient for use in eqn (37) is taken from the standard drag curve for spheres. All properties are evaluated at a film condition defined by taking $r = 1/3$ in eqn (21) and applying it to temperature and mass fraction. For further details, see [12].

The comparison with experimental data begins at the lowest height at which droplet composition is measured. However, for the liquid phase spherical diffusion model,

the results have been found to depend on the shape of the mass fraction profile initially assumed inside the droplet at this point. This profile is estimated as follows. The profile may be assumed to be roughly uniform near the droplet generator tip due to the mixing caused by the droplet formation process. By extrapolating the experimental curves backwards to that point, computation could begin as if that point were the initial condition. When the computation reaches height of the first composition measurement, computed values for droplet diameter, bulk mass ratio, and velocity will in general not agree with the measured values because the extrapolations are not reliable. Therefore, at this point, the computed values are corrected to agree with experimental measurements. The bulk mass ratio is corrected by determining a constant factor which when added to the mass fraction profile at each point in the drop yields the measured bulk mass ratio. Thus the shape of the profile is preserved and is taken to be the best available estimate of the actual shape.

The results of the comparisons for Run 1 are shown in Figs. 30-32. Because the results of the complete mixing assumption are the same as those which would be achieved by allowing thermal and mass diffusivities in the droplet to approach infinity, this model is denoted as "infinite diffusivity" in the figures. The spherical diffusion model is denoted simply as "finite diffusivity". It is seen in Figs. 30 and 31 that the two liquid phase models predict nearly the same acceleration and vaporization rates while at the same time slightly overpredicting both of these. However, in Fig. 32 the liquid phase models are seen to predict significantly different changes in droplet composition, neither of which agrees very well with the data.

It will be recalled that neither liquid phase model was felt to be very realistic. Figure 30 together with the data already reported in [12] and further compared in Volume I, confirms this fact. Furthermore, the fact that the data falls between the predictions of the two models offers strong support for the vortex model discussed in Volume I in which internal mixing does not completely eliminate the effects of diffusion in the droplet.

Recall that Run 1 was the only set of data taken under conditions similar to those in [12]. Because the air temperature in Run 1 was somewhat higher than in [12] and the droplets contained a much greater fraction of n-heptane, direct comparison of the present data with [12] is not straightforward. Nevertheless, the magnitude of the error between the complete mixing model, which was the only liquid phase model considered in [12], and experimental data is roughly of the same order between the two data sets. It is reasonable therefore to believe that the two data sets are consistent.

When extension of the model used above to the conditions of Runs 2-5 was attempted, it was found that vaporization rates were overpredicted by as much as 50%. This error could not be attributed to discrepancies in the liquid phase models or to any known experimental error, so it was concluded that in the lower Reynolds

number range of these experiments, the gas phase model was in error. To check this, it was decided to compare Run 2 with a different gas phase model. Run 2 was chosen because, since the fuel was single component and had an initial temperature equal to the wet bulb temperature, the results of any comparison should be insensitive to the liquid phase model used. This fact was confirmed by comparing the predictions of the previous gas phase model, coupled with each of the liquid phase models. The results were found to be virtually identical, though inconsistent with the data.

The gas phase model used was taken from the work of Renksizbulut and Yuen [6], which is the most recent of experimental works of the stationary droplet variety. The Nusselt number correlation found was

$$(40) \quad Nu = \frac{(2.0 + 0.57 Re^{1/2} Pr^{1/3})}{(1.0 + Bn)^{0.7}}$$

With the exception of the Reynolds number, all properties in eqn (40) are evaluated at a film condition defined by taking $r = 1/2$ in eqn (21) and applying it to temperature and mole fraction. The Reynolds number is evaluated at a mixed film condition given by

$$(41) \quad Re = \frac{S_{\infty} u_{\infty} D}{\mu_b}$$

where the viscosity μ_f is evaluated at the film condition, but the density is evaluated at infinity.

Because the ambient conditions are unsteady in Run 2, the liquid phase is strictly speaking also unsteady. However, if at the initial point the liquid phase is set equal to the wet bulb temperature appropriate for the ambient temperature there, computations have shown that, for this run, further changes in the liquid phase temperature are very small over the measured droplet lifetime, and the energy absorption term q_i'' is negligible compared with the latent heat. Therefore it is a good approximation to treat the liquid phase in Run 2 as steady state. If this is done, the droplet heat and mass fluxes are related through the latent heat as in eqn (9), and eqn (40) is sufficient to completely describe the overall vaporization process.

In Figures 33 and 34, the new gas phase model is compared with Run 2. Shown

also are the predictions of the previous gas phase model. In both cases, the complete mixing assumption is used in the liquid phase, and the drag correlation used in the standard drag curve for spheres. In Fig. 33, it should be noted that the slight negative curvature evident in the experimental curve fit at larger values of time is a result of the curve fitting technique combined with experimental scatter, and is not considered to be physically realistic. Figure 34 shows that the new gas phase model offers a significantly improved prediction of the droplet vaporization rate. The predictions of droplet acceleration by both models, which are very close to each other, are shown in Fig. 33 to be somewhat greater than the measured acceleration.

The new gas phase model has not yet been compared with Runs 3-5, because the validity of assuming $q_1'' = 0$ for these runs has not been sufficiently examined. Furthermore, whether or not the assumption is valid, the present requirement that the assumption be made in order to apply the model represents a rather restrictive limit on its applicability. An independent Sherwood number correlation consistent with eqn. (40) would eliminate the requirement to neglect q_1'' by providing a means by which its value can be determined. Such a correlation has been reported in [17], which was the source work for [6]. Its incorporation into the above comparisons is currently being studied. Finally, although the model has been shown to predict experimental data significantly better than the previous model, the effects of the existing errors need to be assessed. For example, if droplet acceleration predictions are improved, it is conceivable that vaporization rate predictions could worsen. These considerations are being looked into.

Runs 3-5 have been compared with the previous gas phase model. Vaporization rates continue to be significantly overpredicted. Also, the difference between the results of the two liquid phase models in predicting the change in droplet composition remains large as in Run 1. In the absence of significant gas phase agreement, however, quantitative comparison of liquid phase behavior is not meaningful.

Conclusions

Rates of vaporization and acceleration have been measured for single and multicomponent droplets vaporizing freely in a hot, convective environment having Reynolds numbers in the range $10 < Re < 200$. A generalized method of comparing the data with the predictions of various gas and liquid phase models of droplet vaporization has been outlined. Some limitations of the film property approach for evaluating various properties for use in these models have also been examined. Composition measurements of the droplets support the liquid phase vortex model described in Volume I.

The data has been compared with the same gas phase model which was compared with previous data obtained by this experiment. For the one experiment in which conditions were similar to previous experiments, the amount of agreement was found to be similar. For all other experiments, which were performed in a lower Reynolds number range, vaporization rates were found to be significantly overpredicted. When a different gas phase model due to Renksizbulut and Yuen [6] was compared with a set of single component droplet data chosen to minimize the influence of the liquid phase, agreement was found to have been significantly improved, though still less than perfect. Work on this model is continuing.

It is not necessarily surprising that the gas phase model of [12] does not extend to lower Reynolds numbers. There is no reason to believe that a spherically symmetric theory developed for a constant property stagnant gas phase and corrected for convection by the correlation of Ranz and Marshall, which was obtained from data restricted to low mass transfer rates, to be physically appropriate. The agreement found in [12] between this model and the data obtained there may be no more than the result of a well chosen film property factor r .

This suggests that the film property factor can be viewed as an important tuning parameter in adjusting the predictions of vaporization models. By a choice of $r = 1/3$, the data of [12] could be made to agree with eqn. (39), but there was no guarantee that the agreement could be maintained over a very much wider range of vaporization conditions. Note that eqn. (39) has never been compared with the experimental data of other researchers. By choosing a different value of r , it is probable that the form of eqn. (39) can be made to fit the data of the present study as well.

The use of the film property factor r as a tuning parameter is evident in the work of other researchers. Witness the conflicting recommendations for its value found in the literature. It is not to be implied, however, that using r in this way is always undesirable. For appropriate choices of r , Nusselt and Sherwood number correlations having the general form of eqns. (2) and (3) can be made to fit a wide range of data. Equation (40) is such a correlation. In fact, since empirical correlations are almost always limited in the range of application by the form of the correlation assumed,

the range of application may in some cases be more restricted by this form than by film property considerations. Finally, such tuning can be useful when the gas phase behavior is not of primary concern. In [12], for example, where the emphasis was on the liquid phase behavior of multicomponent droplets, discrepancies in the gas phase behavior could be removed by a series of calibration experiments performed on single component droplets. The effect of various liquid phase models could then be assessed more or less independently.

What should be implied is that the question of a proper choice for the film property condition needs to be more completely examined. It needs to be resolved whether a consistent rule for defining r can be made to represent the majority of existing data. If it cannot, the whole film property concept, at least as represented by the simple form of eqn. (21), may be untenable. Furthermore, if it cannot, the question arises whether the experiments which have been conducted to date have all been consistent. It is possible that some as yet unregulated or unmeasured factor accounts for relatively significant differences in droplet vaporization behavior. One such factor which comes to mind is the degree of purity of the liquid fuel. It is also possible that this factor could change significantly between stationary droplet experiments and free droplet experiments. Extrapolation of the results between the two could then become unreliable.

Future work should therefore further address the film property question. Differences in data obtained from various droplet vaporization experiments, free and stationary, need to be reconciled. To assess the behavior of the liquid phase in the lower Reynolds number range represented by the present experimental data, gas phase predictions of droplet vaporization and acceleration rates need to be made to more closely agree with the data. This will probably require one or two additional single component data sets to be used for calibration. Finally, more free droplet experiments need to be performed at all ranges of Reynolds and mass transfer numbers both to shed more light on liquid phase processes and to compliment the existing body of stationary droplet vaporization data.

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Nomenclature

B	-	Mass transfer number for heat transfer
B_m	-	Mass transfer number for mass transfer
C_D	-	Drag coefficient
C_p	-	Specific heat
D_p	-	Droplet diameter
D	-	Mass diffusivity, m^2/sec
e_s	-	Energy flux at droplet surface
g	-	Gravitational acceleration
k	-	Thermal conductivity
Le	-	Lewis number
L	-	Latent heat
M	-	Molecular weight
m	-	Mass
m''	-	Average mass flux at droplet surface
Nu	-	Nusselt number
q_i''	-	Average heat flux absorbed by droplet which does not directly contribute to vaporization
q_s''	-	Average diffusive component of energy flux at droplet surface
R	-	Droplet radius
r	-	Factor in film property calculation; also radial distance
Sh	-	Sherwood number
T	-	Temperature
t	-	Time
V	-	Droplet velocity
V	-	Air velocity
X	-	Mole fraction; also distance in the test section
Y	-	Mass fraction of fuel
α	-	Thermal diffusivity, m^2/sec
ρ	-	Density
ϕ	-	General property

Subscripts

a	-	Fuel component in droplet of lightest molecular weight
air	-	Air
f	-	Film condition
h	-	Heat transfer
l	-	Liquid phase
m	-	Mass transfer
o	-	Initial condition
s	-	Droplet surface
t	-	Total (mass)
∞	-	Ambient condition

Superscripts

- Affected by q_1''
- Flux: flow rate per unit area

Figure 1

290

DROPLET GENERATOR

Figure 2

OPTICAL SYSTEM

Figure 3

DROPLET COLLECTION PROBES

Figure 4

AERODROPLET COLLECTION PROBE

Figure 5

EXPERIMENTAL APPARATUS VIEW FROM TOP

Figure 6

AIR TEMPERATURE VS. HEIGHT

Figure 7

AIR VELOCITY VS. HEIGHT

Figure 8

DIAMETER VS. HEIGHT

COMPOSITION VS. HEIGHT

Figure 10

DROPLET TRAJECTORY

Figure 11

DIAMETER RATIOS

Figure 12

AIR TEMPERATURE VS. HEIGHT

Figure 13

AIR VELOCITY VS. HEIGHT

Figure 14

DIAMETER VS. HEIGHT

Figure 15

DROPLET TRAJECTORY

Figure 16

Figure 17

AIR TEMPERATURE VS. HEIGHT

Figure 18

AIR VELOCITY VS. HEIGHT

Figure 19

DIAMETER VS. HEIGHT

Figure 20

DROPLET TRAJECTORY

AIR TEMPERATURE VS. HEIGHT

AIR VELOCITY VS. HEIGHT

DIAMETER VS. HEIGHT

Figure 24

DROPLET TRAJECTORY

Figure 25

AIR TEMPERATURE VS. HEIGHT

Figure 26

AIR VELOCITY VS. HEIGHT

Figure 27

DIAMETER VS. HEIGHT

Figure 28

DROPLET TRAJECTORY

Figure 29

DROPLET TRAJECTORY

TIME (MSEC)

Figure 30

DIAMETER VS. HEIGHT

Figure 31

COMPOSITION VS. HEIGHT

Figure 32

DROPLET TRAJECTORY

Figure 33.

Figure 34