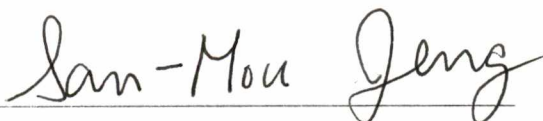


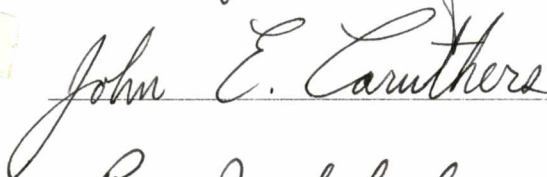
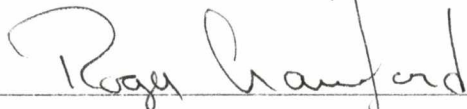
To the Graduate Council:

I am submitting herewith a dissertation written by Louis M. Larosiliere entitled "Bipropellant Spray Combustion Modeling in Small Rocket Engines." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Aerospace Engineering.



San-Mou Jeng, Major Professor

We have read this dissertation
and recommend its acceptance:



Accepted for the Council:



The Graduate School

**BIPROPELLANT SPRAY COMBUSTION MODELING
IN SMALL ROCKET ENGINES**

A Dissertation

Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

Louis M. Larosiliere

December 1991

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ABSTRACT

A CFD-based model for bipropellant spray combustion in small rocket engine combustors is formulated and developed into a predictive computational tool. This model is comprised of a two-component interacting liquid phase imbedded within a turbulent chemically reactive gas. A self-consistent mathematical description is formulated for the liquid and gas phases. The liquid phase is assumed to be composed of two immiscible collections of quasi-spherical material volumes call "globules". This allows a conservation equation similar to the well-known spray equation to be formulated for the globule number density distribution. A pair of unlike globules are allowed to interact through impingement collision which results in a collision induced oscillation of the globule surface. The amplitude of the oscillation can cause the globule surface to deform and eventually breakup into spray droplets. Thus, a simulation of the gross effects of atomization via impinging liquid streams is possible. Furthermore, secondary breakup due to aerodynamic forces are also included. Various other sub-models are developed for droplet combustion, and spray/wall collision. State-of-the-art sub-models are employed for globule acceleration, turbulence dispersion, and spray droplet coalescence. The conservation equations for a continuum gas with imbedded condensed liquid phase elements are derived via a formal averaging procedure. This leads to a consistent form for the interphase exchange rates between the liquid and gas phases. A standard $k-\epsilon$ turbulence

model along with a gas phase chemistry model are incorporated.

The formulated model is integrated within the computational framework of the KIVA-II reactive flow code. An efficient coupling of the various sub-models with the ALE scheme is obtained. A brief outline of this procedure is provided.

Applications to three problems related to small bipropellant spray rocket combustion are demonstrated. A simulation of the spray structure from a like-doublet impinging stream injector is presented. The computed spray structures showing the effects of impingement angle and injection velocity compare favorably with photographs taken by Heidmann. Atomized drop sizes are matched with the correlation of Dickerson. Unlike-doublet stream impingement is also presented for N_2H_4 and N_2O_4 in a confined chamber. The spray/wall impingement flow structure is appraised. Simulations of bipropellant spray combustion via an unlike-doublet impinging stream injector are investigated. Two bipropellant systems (N_2H_4/N_2O_4 and N_2H_4/LOX) are studied. Vastly differing combustion characteristics are computed for the two bipropellant systems. Finally, an investigation of the combustion flow structure with a single-element coaxial pintle injector is presented.

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LIST OF SYMBOLS

A	Surface area
c_p	Specific heat at constant pressure
D	Binary diffusion coefficient in Fick's law
e	Sensible internal energy per unit mass
h	Sensible enthalpy per unit mass
Δh_f^0	Heat of formation at a standard reference temperature
$\bar{r}$	Unit dyad
k	Turbulence kinetic energy per unit mass
NP	Number of liquid parcels
NSP	Total number of chemical species
p	Continuum pressure
Pr	Prandtl number
r	Globule spherical radius
Re	Reynolds number
R_u	Universal gas constant
Sc	Schmidt number
T	Continuum temperature
t	Time coordinate
Δt	Time duration
$\mathbf{u}$	Continuum velocity vector

$\mathbf{q}''$	Continuum fluctuation velocity vector
$\mathbf{v}$	Globule velocity vector
V	Volume
$\hat{W}$	Molecular weight
$\mathbf{x}$	Position vector
y	Dummy variable of integration for position vector
y	Globule surface distortion parameter
$\dot{y}$	Globule surface oscillation parameter
Y_m	Mass fraction ($\frac{\rho_m}{\rho}$)
θ_{cone}	Spray cone angle
λ	Thermal conductivity coefficient
μ	Viscosity coefficient
δ	Dirac delta function
δ_{ik}	Kroneker delta
ϵ	Dissipation of turbulence kinetic energy
$\bar{\tau}$	Viscous stress tensor
ρ	Continuum density

Subscripts

bu	Breakup source term
coll	Collision source term
c	Continuous liquid phase (intact liquid)

d	Condensed liquid phase (dispersed liquid)
g	Gas
I	Interface
imp	Impingement
inj	Injection
l	Liquid
m	Specie identification
p	Chemical product
∞	Ambient conditions for drop combustion calculations

Superscripts

C	Gas chemistry source term
S	Spray source term

1 INTRODUCTION

1.1 Problem Description

Given a liquid bipropellant rocket combustor configuration, a computational analysis of the local combustion and flow characteristics is required. Consider the combustion chamber to be a control volume which may vary with time. Let this volume contain a continuous medium and allow a pair of liquid streams to be introduced into it via an injection system. Upon entering this volume, the liquid phases will undergo mutual interactions as well as interactions with the particular medium within the volume. Possible mutual interactions include impingement and liquid phase chemical reactions. The structure of the liquid streams is inherently unstable and once impingement has occurred, a tendency to quickly transition to a condensed liquid phase will set in. This transition process whereby the surface to volume ratio of the liquid is increased is known as atomization. A liquid droplet spray containing a wide spectrum of attributes is thus generated. If an ignition source is provided either internally or externally, the spray droplets will heat up and then vaporize. Subsequently, a combusting spray imbedded within a chemically reacting continuous medium will be spawned. A sketch of the combustion chamber highlighting some of these physical processes is given in Figure 1. The objective of the current effort is to provide an engineering tool for evaluating the spatial and temporal evolution of the aerothermodynamic field

variables (i.e., pressure, temperature, velocity...) within the combustion chamber.

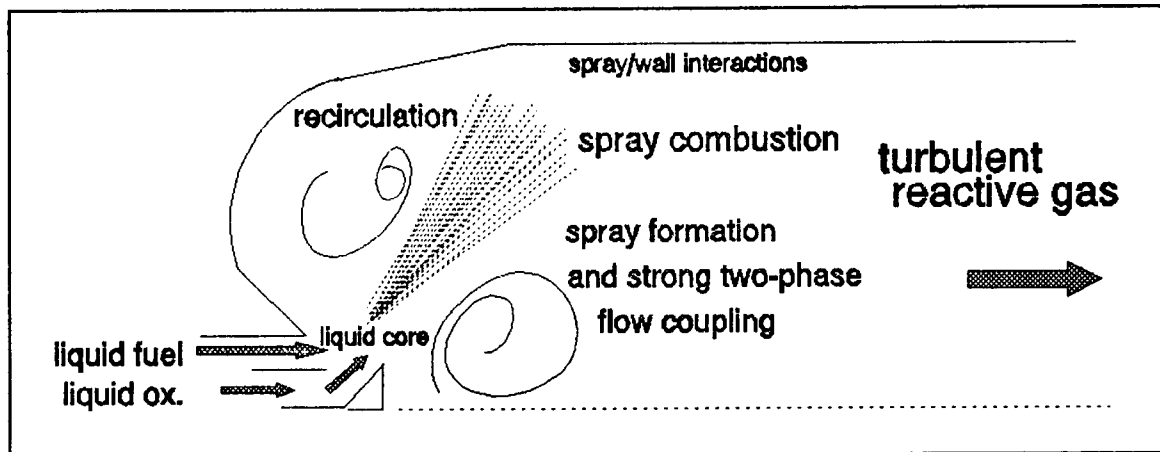


Figure 1. Some critical physical processes in a small liquid bipropellant rocket combustor.

The model to be presented is tailored for the small liquid bipropellant thruster. This class of thrusters has particular needs which will be addressed latter. However, the modelling framework is applicable to a wider class of spray combustion problems. It is hoped that this work will be fruitful as a diagnostic tool for the combustion flow structure in liquid bipropellant rocket thrusters.

1.2 Previous Contributions

The current research extends significantly and applies the work of many previous investigators. Integration of various processes along with sub-processes into an engineering simulation forms the core of this research. Previous contributions are classified into two groups: (1) Those that provide

physical understanding or phenomenological modelling capability for the various processes, and (2) those integrating physical observations within a computational procedure. A background summarization along the lines of these two categories is presented in order to properly position the present effort.

1.2.1 Atomization

Liquid propellants are introduced within the chamber via an injection system. Rocket engine injection systems typically employ multiple elements of like or unlike impinging streams¹. The primary design goal for an injector element is that the injector creates a propellant spray distribution satisfying the goals for performance, chamber and injector durability, and stable combustor operation. One very popular injector element is the unlike-doublet which consists of two cylindrical jets of unlike liquid propellants impinging on each other at a desired angle. A liquid sheet is formed and then breaks up into a droplet spray. The degree of liquid propellant mixing is a function of several variables but an optimum mixing criterion has been formulated by Rupe and Evans¹ based upon experimental non-reactive stream studies. The most uniform mixture ratio spray is produced when the products of fluid density, jet velocity squared, and jet diameter are equal for both streams. A fraction of each stream penetrates the impingement area to reach the other side of the main liquid sheet that is produced. With very reactive propellants, liquid phase reactions in the impinge-

ment region of the jet streams can create enough gaseous products thereby reducing the mixing effectiveness. The gas formation and heat release can cause complete fuel-oxidizer separation to occur resulting in an oxidizer-rich spray on the side of the oxidizer orifice and a fuel-rich spray on the fuel side. Elverum and Staudhammer² first reported that impinging hypergolic liquid streams under certain conditions have a tendency to be blown apart rather than achieve the intended degree of mixing. Burrows³ and Breen et al.⁴ have made photographic observations of the impingement of two hypergolic liquid streams confirming this stream separation tendency. It was shown that the impingement of hydrazine (N_2H_4) and nitrogen tetroxide (N_2O_4) resulted in rapid atomization of the liquid jets but did not produce a homogeneous mixture of fuel and oxidant droplets within the chamber. Tentative criteria to predict the presence or absence of hypergolic stream separation have been advanced by Kushida and Houseman⁵ on the basis of theoretical analysis. Their results revealed that depending on the pressure level, stream separation originated from either liquid/liquid interfacial reactions or gas phase reactions. The physical nature of the separation process, when it did occur, was generally presumed to involve a quasi-steady lamination of the spray fans with fuel on one side and oxidizer on the other (Figure 2). Campbell et al.⁶ demonstrated by way of photography that the hypergolic stream separation phenomenon is a cyclic process in which explosions disrupt the spray fan and drive the jets apart, thereby producing temporary physical separation of fuel and oxidizer. An assessment of either the reactive or non-

reactive stream impingement phenomenon is a necessary step for any predictive methodology.

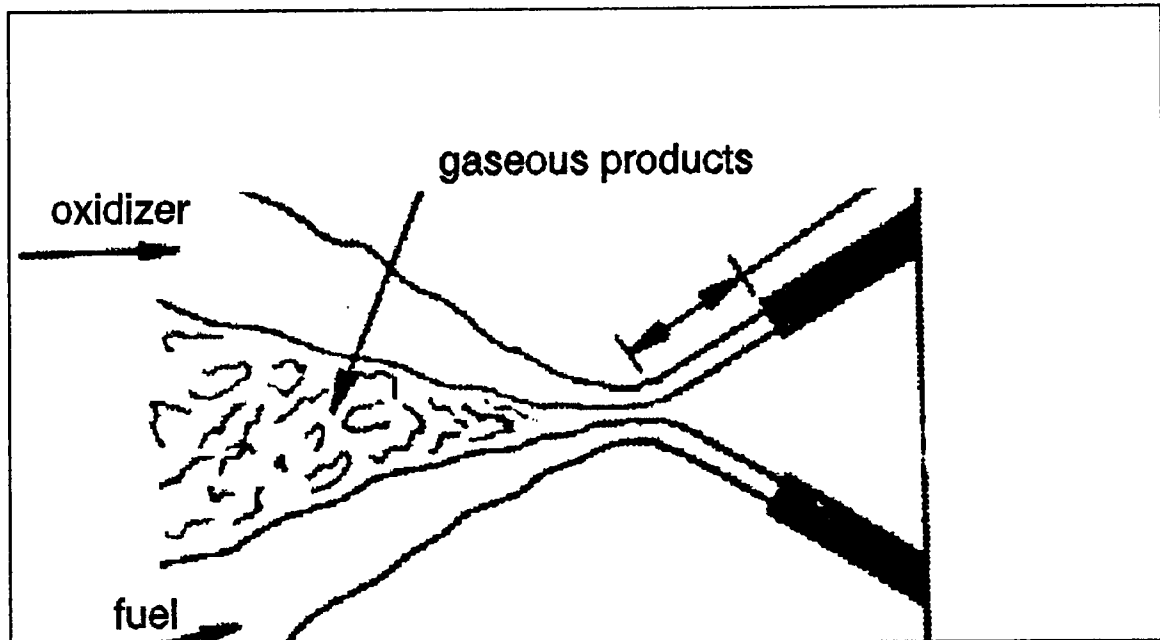


Figure 2. Reactive liquid stream impingement illustrating stream separation phenomenon.

A recent review of atomization in liquid rocket engines was given by Ghafourian⁷. It was concluded that a quantitative predictive ability for atomization still remains elusive. Dombrowski and Hooper⁸ reported that with geometrically similar injectors, the sheet disintegration mechanism depends upon whether the jet is laminar or turbulent. A turbulent jet generally disintegrates under the actions of impact waves produced by impingement whereas a laminar jet can disintegrate under the actions of either impact waves or aerodynamically induced waves. Droplet formation by means of aerodynamically generated waves is fairly well understood⁷. Impact wave disintegration is not widely reported. Heidmann

et al.⁹ showed that the process of liquid sheet disintegration is periodic in its spatial characteristics. They postulated that a condition of unstable equilibrium may occur when external forces tending to breakup the sheet are not balanced by the surface tension and viscous forces within the liquid. Foster and Heidmann¹⁰ showed the existence of spatial variations in the spray pattern created from two impinging jets. Hence, a single property characterizing the entire spray may be inappropriate. There are numerous correlations¹¹ available for the droplet size and distribution from impinging liquid jets. However, most of these correlations are far too simple to be of absolute use. The effects of the local combustion flow structure are not accounted for and the experimental techniques employed are subject to large uncertainties.

Reitz¹² proposed a new atomization modelling method whereby the stability of large liquid drops are simulated from the results of stability analysis for liquid jets. In this model, the liquid is injected as discrete parcels of liquid drops having a characteristic size on the order of the injector orifice diameter. The injected drop's size decreases with time due to breakup and the equilibrium size is specified using experimental drop breakup correlations. Only the inertial effects of the surrounding gas enters into Reitz's model. This approach effectively assumes that the fully developed spray drop size is determined by competition between secondary drop breakup and coalescence. Thus the effects of the injector nozzle are not strongly coupled with the secondary atomization process.

O'Rourke and Amsden¹³ presented a method along the same lines for calculating drop aerodynamic breakup in internal combustion engine sprays. This model is based on an analogy between an oscillating and distorting droplet and a spring mass system. The effects of impact waves and possibly the influence of the injector nozzle can presumably be incorporated within the method of O'Rourke. Numerical simulations of atomization are currently under development. Two basic techniques, the Volume of Fluid¹⁴ (VOF) and Jet-Embedding (JE) have been developed for modeling the two-phase flows with sharp liquid jet interface. These techniques are incapable of providing reliable quantitative results at present.

1.2.2 Spray Analysis

Recent advances concerning the analysis of sprays have been reviewed by Faeth¹⁵. Consideration is given to both dilute sprays which contain more-or-less spherical drops and have relatively small liquid fractions; and dense sprays, which comprise near injector conditions with irregularly shaped liquid elements and relatively high liquid fractions. Three methods have been devised for analyzing dilute turbulent dispersed flows and they are as follows: (1) locally homogeneous flow (LHF) analysis where interphase transport rates are assumed to be infinitely fast; (2) deterministic separated flow (DSF) analysis where finite interphase transport rates are considered but dispersed phase turbulence

interactions are ignored; and (3) stochastic separated flow (SSF) analysis where both finite interphase transport rates and effects of dispersed phase turbulence interactions are considered. According to Faeth, the major unresolved issues for dilute sprays involve turbulent dispersion of drops, modification of continuous phase turbulence properties by drops, and the effect of turbulence on interphase transport rates.

A dense spray intuitively appears to be a close-packed collection of roughly spherical drops, but upon closer look, dispersed phase elements having complex shapes with significant effects of collisions and breakup are involved. Dispersed elements having irregular shapes pose serious conceptual difficulties for separated-flow-analysis of dense sprays. Recent work by Wu¹⁶ suggests that LHF analysis might be effective in the dense spray region. Additional studies are needed to formulate an appropriate model for dense sprays.

Combustion of liquid droplets in a spray is inherently governed by mass and heat transfer mechanisms between the spray and its environment. Both premixed and diffusion flame theories¹⁷ have been applied to spray combustion problems. In very dilute sprays, individual drop burning is prevalent. For dense sprays, Chiu¹⁸ presented the group-combustion model. In this model, the collective behavior of drops is accounted for by a simultaneous analysis of an inner heterogeneous region and an outer homogeneous gas phase region.

Although the group combustion model includes many important aspects of spray combustion, numerous improvements are needed before it can be routinely applied.

Numerical methods for sprays are detailed in the works of Dukowicz¹⁹ and O'Rourke²⁰. Dukowicz suggested that the ideas of the Monte Carlo method could be combined with particle methods for spray calculations. He also provided an efficient technique for coupling the spray source terms with the gas flow. O'Rourke extended this method by including the effects of droplet collisions and coalescence. Sirignano²¹ provided an instructive discussion of the formulations of spray combustion models along with some computational issues. Eulerian, Lagrangian, and probabilistic descriptions of a spray were compared showing the advantages of each with respect to a desired level of resolution. The probabilistic formulation was declared to be the most consistent of the three since it allows for a wide range of resolution of the complex physical phenomena.

1.2.3 Turbulent Chemically Reacting Flows

The ambient medium surrounding the two interacting liquid streams is taken to be a turbulent reactive gas flow. Analysis of even non-reacting turbulent flows has been particularly difficult due to the existence of a wide range of length

and time scales associated with the evolution of the flow. When such flows are reacting, computational difficulties are notoriously enhanced due to the additional complications associated with the evaluation of non-linear reaction rates, large density variations, and coupling between the fluid dynamics and the chemistry. A detailed review of the state-of-the-art in chemically reactive turbulent flows was presented by Giv²². Turbulent flow modelling is categorized into a statistical approach and what is called "Model-Free" simulations. The statistical approach introduces new correlation terms which need to be modelled. Models for these new terms are based on (1) moment methods, and (2) Probability Density Function (pdf) techniques. In the first approach, the transport equations for the correlation terms are constructed; whereas in the second method, the evolution of the pdf of the statistical variables is considered. Moment methods are relatively easy to use in engineering applications and have also proven to be adequate in a lot of situations²³. A disadvantage of the moment methods is that the mean reaction rates are difficult to evaluate due to their highly nonlinear nature. The pdf method allows for the direct evaluation of the mean reaction rate. Despite the attractiveness of the pdf method in obtaining a closed representation of the reaction term, there is a major difficulty with the implementation of the method. This difficulty is that the dimensionality of the pdf increases with the number of the scalars and the number of statistical points considered. The availability of supercomputers has introduced an ability to solve appropriate transport equations of turbulent flows without the need for a priori modeling over

some limited parameter range. Model-Free simulations consist of solving the temporal evolution of the detailed unsteady structures in a turbulent flow field. Presently, there are severe restrictions on the applicability of this method for practical engineering use.

1.2.4 Rocket Combustion Analysis

Most current models for performance analysis of rocket combustion tend to decouple the critical processes. A zonal approach is usually taken whereby different assumed physical processes of interest are modeled and then conveniently connected. Priem and Heidman²⁴ presented the first useful one-dimensional model for rocket engine combustion. The spray and gas phase equations were coupled but constant values were used for chamber pressure and combustion gas properties. Subsequent investigators included axial pressure variation, secondary droplet breakup and bipropellant spray tracking. These one-dimensional steady-state models are relatively easy to use. Required input data include chamber axial crosssections, propellant properties, combustion product composition, and initial spray droplet properties. The initial spray droplet properties provide the only link to the injector design and are the most crucial input data. A purely one-dimensional model is obviously lacking as a local performance diagnostic tool. To rectify this deficiency, some quasi-multidimensional models have been formulated by integrating a number of locally one-

dimensional models. This leads to the JANNAF methodology²⁵ employing such codes as: ODE (one-dimensional equilibrium flow), ODK (one-dimensional kinetic flow), TDK (two-dimensional kinetic flow), and TBL (turbulent boundary layer flow). Such an approach does not resolve the local combustion chamber aerothermodynamics but is effective in predicting overall engine performance and exhaust nozzle two-dimensional flow characteristics if the combustion process is well behaved. Sutton et al.²⁶ described a comprehensive method for analyzing liquid rocket engine combustion. Using continuum mechanics for both gas and liquid spray phases, this method expresses the three-dimensional dynamics of a multicomponent reacting gas stream which undergoes simultaneous exchange of mass, momentum, and energy with contained liquid bipropellant sprays. This approach requires a critical amount of spray initial conditions to be given as external input. Liang et al.²⁷ constructed a computational model for the rocket combustion of H₂ gas and LOX with coaxial injection. They described a comprehensive three-phase (liquid, spray droplets, and gas) model capable of resolving some atomization length and time scales. This model is computationally too intensive for engine development needs and not directly applicable to impinging liquid stream atomizers.

The state-of-the-art in engine spray combustion modelling requires as external input an ample amount of injection system characterization in order to be useful. Recent developments²⁸ in spray combustion modelling aimed at the

gas turbine and internal combustion engine arena have produced a wealth of simulation techniques which haven't yet been fully applied to the rocket engine combustor. Creative exploitation of these techniques for the bipropellant rocket thruster remains to be done.

1.3 Approach

The current research focuses on the development of a fundamental CFD-based modelling approach for analyzing the liquid bipropellant spray combustion and flow evolution in small rocket combustion chambers. A self-consistent physical model is formulated and integrated within the computational framework of the KIVA-IF⁹ chemically reactive flow code developed for internal combustion engines. This formulation attempts to reduce the amount of injection system characterization that is needed in order to specify the spray initial conditions. Emphasis is placed on the "sub-scale" modelling of the injection/atomization process, and the bipropellant gasification modes. These "sub-scale" models and their integration within a CFD method represent a unique contribution to the state-of-the-art in small rocket engine combustion analysis. The model is then applied to a variety of spray combustion related problems in order to illustrate its capabilities.

2 MODEL FORMULATION

2.1 Physical Model

The media being considered consist of a pair of homogeneous liquid phases contained within a continuum gas occupying a prescribed volume. A two-phase flow situation is thus realized. The structure of the liquid phases is inherently unstable due to the sharp density gradient existing at the interface between the gas and liquid. Furthermore, if an atomization mechanism is present, the continuous liquid phase will quickly disintegrate into a condensed liquid phase. Subsequently, this condensed liquid phase will vaporize and generate more gas. Gas phase combustion will propagate and generate a multi-species chemically reacting gas mixture. These events are described by two sets of similar equations, one for the two liquids and another for the gas. The liquid and gas phases are coupled through the interface conditions which represent the interactions of the two phases. These interactions are exchanges of mass, momentum, energy, and species across common interfaces. Moreover, the liquid phase may be composed of two immiscible components interacting through a liquid material interface. Interactions among the two immiscible components of the liquid phase occur as a result of collisions.

Having two sets of equations, one for each phase, it is possible to attempt

a numerical solution. The spatial and temporal resolutions required to produce a numerical solution capable of directly describing all the processes taking place are too great for any current computer. Therefore, "subscale" models of processes not numerically resolvable are necessary. Processes which are not numerically resolvable in the present analysis are: liquid stream impingement/collisions, atomization, droplet combustion, turbulence, and chemical kinetics. Sub-models for these processes will be incapable of giving a priori local details, but should provide phenomenological descriptions of observable critical processes. A self-consistent formulation capable of directly absorbing these sub-models is established in what follows.

2.2 Conservation Concept

Physical conservation only has meaning over a finite region of space during a finite time interval. According to Truesdell⁸⁰, a general conservation rule may be represented in the classical sense as:

$$\int_{V(t_2)} U \, dV - \int_{V(t_1)} U \, dV + \int_{t_1}^{t_2} \oint_{A(t)} \mathbf{F} \cdot \mathbf{n} \, dA \, dt = \int_{t_1}^{t_2} \int_{V(t)} P \, dV \, dt, \quad (2.1)$$

where U is a conserved variable, $\mathbf{F}$ is a flux term containing both convective and non-convective parts, and P is a production source term. This conservation rule is applicable to either the liquid or gaseous phases. If all variables are continuous in time, equation (2.1) can be written as:

$$\frac{d}{dt} \int_{V(t)} U dV + \int_{A(t)} \mathbf{F} \cdot \hat{n} dA = \int_{V(t)} P dV . \quad (2.2)$$

This conservation concept will be implemented separately for each phase.

2.3 The Liquid Phase

The liquid phase consists of a two-component immiscible liquid mixture. Within the liquid phase, two characteristic regimes are identified as an intact liquid core and a dispersed liquid cluster. The intact liquid core is comprised of continuous liquid columns, sheets, and ligaments. A dispersed liquid cluster contains both dilute and dense distributions of condensed liquid elements. These two regimes are connected in the sense that the origin of the dispersed liquid cluster can be traced back to the breakup of the intact liquid core. Of prime interest here is calculating the initial conditions for the dispersed liquid cluster (i.e., spray) which is produced by the interaction of two continuous liquid streams. It is assumed that a continuous liquid stream is the limiting case of a highly dense collection of quasi-spherical liquid material volumes call "globules". The surface of a globule can undergo distortions and oscillations resulting in the breakup of the globule into droplets of smaller sizes. This idealization is not substantiated but it is invoked due to its conceptual and mathematical simplicity. Conceptually, this allows the entire liquid phase to be cast within a separated flow (SF) formulation for a collection of globules. The size of a globule is taken

to be a characteristic length (i.e., diameter) of the orifice from which it is injected.

Let $\mathcal{S}$ be a vector of variables describing the state of a globule at a certain time. A globule number density distribution function $F(\mathcal{S}, t)$ is defined in such a way that $F(\mathcal{S}, t) d\mathcal{S}$ gives a measure of the number of globules with attributes in the range $d\mathcal{S}$ about $\mathcal{S}$ at time t . It is postulated that the globule number density distribution is a conserved variable. Hence, equation (2.1) may be adapted for this distribution function in the form:

$$\int_{\mathcal{S}(t_2)} F(\mathcal{S}, t_2) d\mathcal{S} - \int_{\mathcal{S}(t_1)} F(\mathcal{S}, t_1) d\mathcal{S} = \int_{t_1}^{t_2} \int_{\mathcal{S}(t)} \dot{F}_{coll} d\mathcal{S} dt + \int_{t_1}^{t_2} \int_{\mathcal{S}(t)} \dot{F}_{bu} d\mathcal{S} dt . \quad (2.3)$$

This equation relates the net change in globule number over a globule state during a finite time interval to net production by collisions and breakup. If the mutual interactions between the two liquid streams do not produce any new liquid species, then

$$F(\mathcal{S}, t) = F_1(\mathcal{S}, t) + F_2(\mathcal{S}, t) .$$

For applications of interest, $\mathcal{S}$ is taken to be:

$$\mathcal{S} = \left\{ \begin{array}{c} x \\ v \\ r \\ y \\ \dot{y} \\ T_d \\ \theta \end{array} \right\}$$

where x is the physical position of a globule, v is the velocity of a glob-

ule, r is the equilibrium spherical radius of a globule, and T_d is a globule's temperature (assumed to be uniform within a globule). The liquid continuum mass density is assumed constant. Postulating that at any spatial location, the liquid phase exists in the form of either an intact liquid core or a dispersed liquid cluster, but not both, then:

$$\theta = \lim_{V_l \rightarrow 0} \frac{V_c}{V_c + V_d} ,$$

where θ takes on integral values of either zero for the dispersed liquid cluster or one for the intact liquid. Thus, θ serves as a marker identifying the two liquid phase regimes. The total liquid volume, V_l , consists of either the intact liquid core volume V_c , or the dispersed liquid volume V_d . Similar to O'Rourke¹³, the state of the fundamental mode of distortion, y and that of oscillation, $\dot{y}$ of the globule surface are included as parameters. These parameters will be described latter when the globule breakup model is formulated.

Decomposing the two liquid streams into intact liquid cores and dispersed liquid clusters gives:

$$F_1(\mathcal{S}, \eta) = \theta g_1(\mathcal{S}, \eta) + (1 - \theta) f_1(\mathcal{S}, \eta) , \quad (2.4)$$

$$F_2(\mathcal{S}, \eta) = \theta g_2(\mathcal{S}, \eta) + (1 - \theta) f_2(\mathcal{S}, \eta) . \quad (2.5)$$

These two equations (2.4 and 2.5) state that each specie of the liquid phase consists of an intact liquid core with a globule number density distribut-

ion $g(\mathcal{S}, \eta)$, and a dispersed liquid cluster with a number density distribution $f(\mathcal{S}, \eta)$. It is assumed that the intact liquid core is spatially independent of the dispersed liquid. Therefore, both dispersed liquid and intact liquid satisfy equation (2.3) but at different locations in the liquid globule state space. The intact liquid transitions to the dispersed liquid by a breakup mechanism. For a continuous time interval, the globule number conservation for the entire liquid becomes:

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{S}(\eta)} \theta g(\mathcal{S}, \eta) d\mathcal{S} + \frac{d}{dt} \int_{\mathcal{S}(\eta)} (1-\theta) f(\mathcal{S}, \eta) d\mathcal{S} = \\ \int_{\mathcal{S}(\eta)} \theta \dot{g}_{coll} d\mathcal{S} + \int_{\mathcal{S}(\eta)} (1-\theta) \dot{f}_{coll} d\mathcal{S} + \\ \int_{\mathcal{S}(\eta)} \theta \dot{g}_{bu} d\mathcal{S} + \int_{\mathcal{S}(\eta)} (1-\theta) \dot{f}_{bu} d\mathcal{S} . \end{aligned} \quad (2.6)$$

It should be noted that the derivative $\frac{d}{dt}$ is a time rate of change along a globule characteristic path in the globule state space. Hence, convective fluxes do not appear explicitly. The well-known transport theorem³⁰ can be employed to obtain an explicit expression containing the convective fluxes due to the rate of change of the globule state variables. Furthermore, as θ discretely switches to either zero or one, separate equations applicable in the intact liquid core and the dispersed liquid cluster may be obtained. Letting θ be equal to one in equation (2.6) gives for the intact liquid:

$$\frac{d}{dt} \int_{S_i(t)} g_i(\mathbf{S}_i, t) d\mathbf{S}_i = \int_{S_i(t)} \dot{g}_{coll,i} d\mathbf{S}_i + \int_{S_i(t)} \dot{g}_{bu,i} d\mathbf{S}_i \quad (2.7)$$

$i=1, 2$.

Similarly, letting θ be equal to zero gives for the dispersed liquid cluster:

$$\frac{d}{dt} \int_{S_d(t)} f(\mathbf{S}_i, t) d\mathbf{S}_i = \int_{S_d(t)} \dot{f}_{coll,i} d\mathbf{S}_i + \int_{S_d(t)} \dot{f}_{bu,i} d\mathbf{S}_i . \quad (2.8)$$

Equations (2.7) and (2.8) are similar in form but different in content. The differences are due to the characteristics of the breakup and collision source terms within the two regimes. These two equations are coupled in the sense that the intact liquid core supplies the initial conditions for the dispersed liquid cluster. Within the dispersed liquid cluster, the exact location of the individual droplets resulting from globule breakup will not be known for most practical spatial discretizations. In that case, the function $f(\mathbf{S}_i, t)$ in equation (2.8) should be viewed in terms of the probability of finding a droplet in a unit volume of the droplet state space. The two intact liquid cores undergo deterministic processes such as impingement and breakup. Globule breakup results in a probabilistic distribution for the product droplet properties. Thus, the overall situation involves one whereby a deterministic continuous liquid core transitions to a stochastic dispersed liquid cluster evolving within a gaseous medium. The gas phase influences the liquid globules through the evolution of the globule state variables. To close the liquid phase formulation, the collision and breakup source terms must be modelled along with the evolution of the state variables (i.e., $\frac{d\mathbf{S}(t)}{dt}$).

2.4 Averaging Concepts

In this analysis, interest is focused upon the average behavior in space and time of certain properties of the liquid and gas phases. For the present formulation, the liquid phase has been cast into an SF formulation thereby constraining the structure of the liquid/gas interface. Information about the interface is contained in the globule distribution function. The gas phase is distributed over a continuum volume populated by a non-uniform distribution of liquid globules. Averaging the gas phase conservation equations over this continuum volume allows a description of the average gas phase properties without considering the local details of the gas /liquid interface.

The averaging starts by introducing a weighting function³¹ which may be regarded as arbitrary apart from the following conditions: (1) $w(\vec{x})$ has continuous first partial derivatives with respect to $\vec{x}$, (2) $w(\vec{x})$ is normalized so that

$$\int_{-\infty}^{+\infty} w(\vec{x}) d\vec{x} = 1 .$$

The two-phase flow is essentially unsteady and three-dimensional in its detailed structure. An ensemble averaging over many occurrences is employed for the temporal fluctuations. The average number of globules n with certain attributes

in the range $\Delta \mathcal{S}$ about $\mathcal{S}$ is defined as:

$$F(\mathcal{S}, \Delta \mathcal{S}) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N n(\mathcal{S}, \Delta \mathcal{S}, t, \gamma) , \quad (2.9)$$

where N is the number of occurrences γ over which significant changes are observed. The media occupy complementary volumes V_g and V_l at any time. A gas volume or void fraction is introduced as

$$\theta_g(\mathcal{X}, \mathcal{H}) \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{V_g(t, \gamma)} w(\mathcal{Y} - \mathcal{X}) d\mathcal{Y} \quad (2.10)$$

where $V_g(t, \gamma)$ is the volume occupied by the gas at time t in occurrence γ . Equation (2.10) can also be written as

$$\theta_g(\mathcal{X}, \mathcal{H}) = 1 - \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{V_l(t, \gamma)} w(\mathcal{Y} - \mathcal{X}) d\mathcal{Y} . \quad (2.11)$$

where $V_l(t, \gamma)$ is the volume occupied by the liquid. The liquid is now idealized as a collection of globules. If the globules in an event are divided into classes, with globules in a particular class having properties in the range $(\mathcal{S}, \mathcal{S} + \Delta \mathcal{S})$, then the void fraction can be shown³² to be:

$$\theta_g(\mathcal{X}, \mathcal{H}) = 1 - \sum_{i=1}^2 \int \frac{4}{3} \pi r_i^3 w(\mathcal{Y} - \mathcal{X}) F_i(\vec{\zeta}_i, \mathcal{Y}, \mathcal{H}) d\mathcal{Y} d\vec{\zeta}_i , \quad (2.12)$$

where,

$$\vec{\zeta} = \left\{ \begin{matrix} r \\ \vec{r} \\ y \\ \dot{y} \\ T_d \\ \theta \end{matrix} \right\} .$$

Hence, the weighting function $w(\vec{x})$ determines the extent of the spatial influence of a globule distribution at a given point in physical space. In Ref. 32, the weighting function is constructed in such a way that

$$\int w(\vec{y}-\vec{x}) F(\vec{\zeta}, \vec{y}, t) d\vec{y} = F(\vec{\zeta}, \vec{x}, t) .$$

This effectively requires the weighting function to behave like a Dirac distribution. In what follows, the weighting function will be taken to fall off rapidly to zero away from the control point $\vec{x}$. Thus, the influence of the globule distribution on relatively remote points is assumed negligible.

Two averages are defined in terms of the weighting function as follows:
the intrinsic average,

$$\langle \psi(\vec{x}, t) \rangle = \frac{1}{\theta_g(\vec{x}, t)} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{V_g(t, \gamma)} w(\vec{y}-\vec{x}) \psi(\vec{y}, t, \gamma) d\vec{y} , \quad (2.12)$$

and the non-intrinsic average,

$$\bar{\psi}(\vec{x}, t) = \theta_g(\vec{x}, t) \langle \psi(\vec{x}, t) \rangle . \quad (2.13)$$

The intrinsic average gives the average value of a property in the gas

phase, whereas the non-intrinsic average is the average of a property over the entire continuum volume (i.e., both liquid and gas). Intuitively, the significance of the non-intrinsic average is that of a bulk average formed without regard to the concentration of the medium in question. If ψ is any property per unit mass of the gas phase, the density weighted average value is defined as

$$\bar{\psi}(x,t) = \frac{\overline{\rho\psi}}{\bar{\rho}} . \quad (2.14)$$

The fluctuation about the average value is defined by

$$\psi'' = \psi - \bar{\psi} \quad ; \quad \psi' = \psi - \bar{\psi} . \quad (2.15)$$

It is assumed that the average (intrinsic or non-intrinsic) of the fluctuations is zero. Application of Leibnitz's rule and the divergence theorem along with the properties of the weighting function leads to (see Ref. 31):

$$\frac{\partial \bar{\psi}}{\partial x_i} = \frac{\partial \bar{\psi}}{\partial x_i} - \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_i(t,\gamma)} w(\gamma-x) \psi(\gamma,t,\gamma) n_i dA(\gamma) , \quad (2.16)$$

and,

$$\frac{\partial \bar{\psi}}{\partial t} = \frac{\partial \bar{\psi}}{\partial t} + \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_i(t,\gamma)} w(\gamma-x) \psi(\gamma,t,\gamma) \nabla_s \cdot \hat{n} dA(\gamma) . \quad (2.17)$$

The variable ∇_s is the surface velocity of the local liquid/gas interface with surface area A_i having a unit normal $\hat{n}$. Equation (2.16) relates the intrinsic average of the gradient of an instantaneous gas phase variable to the gradient of its intrinsic averaged value and an interface averaged contribution. An

analogous interpretation can be given to equation (2.17) in terms of the flux of a property across the interface. These results will be needed when carrying out the averaging process.

2.5 The Averaged Gas Phase Equations

The local field description for the gas phase can be obtained by applying the conservation statement (eq. 2.1) to an infinitesimal control volume encompassing only gas. A generalized form for the local gas phase equations can be written as:

$$\frac{\partial \psi}{\partial t} + \vec{\nabla} \cdot (\psi \vec{u} - \vec{\Omega}) = \sigma, \quad (2.18)$$

where ψ is any gas phase conserved variable. The variable $\vec{\Omega}$ accounts for non-convective fluxes and σ is a relevant source term. Taking the non-intrinsic average of equation (2.18) and using equations (2.16) and (2.17) result in:

$$\frac{\partial \bar{\psi}}{\partial t} + \vec{\nabla} \cdot (\bar{\psi} \vec{u} - \vec{\Omega}) = \bar{\sigma} + \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_\gamma(t, \gamma)} w(\vec{y} - \vec{x}) [\psi (\vec{u} - \vec{v}_s) - \vec{\Omega}] \cdot \hat{n} dA. \quad (2.19)$$

Equation (2.19) is similar in form to equation (2.18) except for the appearance of an added source term accounting for the existence of the liquid/gas interface. This equation is adapted for each of the gas phase conserved variables. It should be noted that by employing the non-intrinsic average, there is no longer any quantity to indicate the porosity of the two-phase media. This implies that the

density ρ is not just the gas mass per unit gas volume but a gas mass distributed over the entire continuum volume. This difference between continuum density and gas density is expected to be very small when the volume occupied by the liquid phase is not significant compare to the total volume (i.e., $\theta_g \gg 0$).

Averaged gas phase species mass conservation

The species mass continuity equation in a multicomponent gas mixture is derived from equation (2.19) with ψ replaced by ρY_m (i.e., species mass per unit volume) under the assumptions of Fick's law of binary diffusion. After some algebraic manipulations³¹, the following is obtained*

$$\frac{\partial \bar{\rho} \tilde{Y}_m}{\partial t} + \frac{\partial \bar{\rho} \tilde{Y}_m \tilde{u}_k}{\partial x_k} = \frac{\partial}{\partial x_k} \left[\bar{\rho} D \frac{\partial \tilde{Y}_m}{\partial x_k} - \bar{\rho} \widetilde{Y_m'' u_k''} + \bar{\rho} \widetilde{D''} \frac{\partial \tilde{Y}_m''}{\partial x_k} \right] + \bar{\dot{\rho}}_m^c + \bar{\dot{\rho}}_m^s \quad (2.20)$$

$$m=1,..NSP ; k=1,..3$$

where,

$$\begin{aligned} \bar{\dot{\rho}}_m^c &= \text{chemical mass production ,} \\ \bar{\dot{\rho}}_m^s &= \text{liquid-gas interfacial mass production .} \end{aligned}$$

The liquid to gas interfacial mass production is determined by

* Summation convention over repeated indices is implied.

$$\dot{\rho}_m^s = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_I} w(\gamma-x) [\rho Y_m (u_k - v_{s,k}) - \rho D \frac{\partial Y_m}{\partial x_k}] n_k dA(\gamma) , \quad (2.21)$$

where the integral⁺⁺ represents a material fluxing across the liquid/gas interface (A_I). The chemical source term is obtained from the gas phase chemistry model to be described in the next section. Summing equation (2.20) over all species gives the mixture continuity equation as:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_k}{\partial x_k} = \sum_{m=1}^{NSP} \dot{\rho}_m^s = \dot{\rho}^s . \quad (2.22)$$

Averaged gas phase momentum equation

The momentum equation is obtained from equation (2.19) with a Newtonian constitutive relation for the stress tensor. Neglecting body forces, the momentum equation is

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_k}{\partial x_k} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_k} [\bar{\tau}_{ik} - \bar{\rho} \widetilde{u_i'' u_k''}] + F_i^s , \quad (2.23)$$

where,

$$F_i^s = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_I} w(\gamma-x) [\rho u_i (u_k - v_{s,k}) + p \delta_{ik} - \tau_{ik}] n_k dA(\gamma) , \quad (2.24)$$

and

⁺⁺ All variables within the integral are functions of space, time, and event γ .

$$\tau_{ik} = \mu \left[\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right] - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} . \quad (2.25)$$

Equation (2.24) accounts for the momentum transfer across the liquid/gas interface and depends upon processes occurring in the vicinity of this interface.

Averaged gas phase internal energy

The gas phase internal energy balance neglects Soret and Dufour effects. This amounts to assuming that thermal diffusion, body forces, and pressure gradient induced diffusions are negligible. From equation (2.19) and the first law of thermodynamics with Fourier's heat conduction law, the averaged internal energy balance for a gas mixture is:

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{e} \tilde{u}_k}{\partial x_k} = & - \bar{\rho} \frac{\partial \tilde{u}_i}{\partial x_i} + \tau_{ik} \frac{\partial \tilde{u}_i}{\partial x_k} - \frac{\partial}{\partial x_k} [\bar{q}_k + \bar{\rho} \widetilde{e'' u_k''}] - \\ & \bar{\rho} \frac{\partial u_i''}{\partial x_i} + \frac{\tau_{ik} \partial u_i''}{\partial x_k} + \bar{\dot{Q}}^c + \bar{\dot{Q}}^s , \end{aligned} \quad (2.26)$$

where,

$$\begin{aligned} \bar{\dot{Q}}^c &= \text{chemical heat release rate} , \\ \bar{\dot{Q}}^s &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_\gamma} w(\gamma - \bar{x}) [\rho \alpha(u_k - v_{s,k}) + q_k] n_k dA(\gamma) , \\ q_k &= -\lambda \frac{\partial T}{\partial x_k} - \rho D \sum_{m=1}^{NSP} h_m \frac{\partial Y_m}{\partial x_k} . \end{aligned} \quad (2.27)$$

The averaged internal energy $\tilde{e}$ in equation (2.26) is the sensible thermal energy excluding contributions from chemical reactions. Thermal energy exchanges near

the liquid/gas interface are acknowledged by the source term $\dot{Q}^S$.

Averaged fluctuation kinetic energy

The fluctuation kinetic energy per unit mass (KE) is defined by

$$q'' = \frac{u_i'' u_i''}{2}.$$

An equation for the averaged fluctuation KE can be derived by manipulating the averaged momentum and continuity equations (see Appendix) to obtain:

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{q}''}{\partial t} + \frac{\partial \bar{\rho} \bar{q}'' \bar{u}_k}{\partial x_k} &= \frac{\partial \bar{\tau}_{ik} u_i''}{\partial x_k} + \bar{p} \frac{\partial u_i''}{\partial x_i} - \frac{\partial \bar{\rho} \widetilde{q'' u_k''}}{\partial x_k} - \\ &\quad \bar{\rho} \widetilde{u_i'' u_k''} \frac{\partial \bar{u}_i}{\partial x_k} - \frac{\partial \bar{p} u_i''}{\partial x_i} - \bar{\tau}_{ik} \frac{\partial u_i''}{\partial x_i} + \dot{W}^S, \end{aligned} \quad (2.28)$$

where

$$\begin{aligned} \dot{W}^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \int_{A_i} w(\vec{y}-\vec{x}) & \left[\bar{\rho} \frac{u_i u_i}{2} (u_k - v_{s,k}) + \bar{p} u_k - \bar{\tau}_{ik} u_i \right] n_k dA(\vec{y}) - \bar{u}_i F_i^S + \\ & \frac{\bar{u}_i \bar{u}_i}{2} \dot{\rho}^S. \end{aligned} \quad (2.29)$$

Equation (2.28) explicitly shows how the gas phase turbulence is produced, modulated, and transported within a two-phase flow. The term $\dot{W}^S$ accounts for the transport of kinetic energy and work done by stresses at the interface.

2.6 Liquid/Gas Interface Conditions

The local liquid/gas interface conditions are obtained by integrating equation (2.2) over a thin slab containing both liquid and gas and letting the volume of this slab tend to zero. In the limit, the integrals over the interface are composed of two parts, namely integrals over each face of the slab. Performing this exercise leads to:

$$\int_{A_i} [\mathbf{F}_+ - \mathbf{F}_-] \cdot \hat{\mathbf{n}}_+ dA = \lim_{V \rightarrow 0} \int_V P dV - \lim_{V \rightarrow 0} \frac{d}{dt} \int_V U dV, \quad (2.30)$$

where we have arbitrarily chosen one face as the "positive" side of the slab, identifying quantities on this side by the subscript + and those on the other side by the subscript -. Equation (2.30) is now specialized for the different conserved variables.

Species interface condition

Employing the interface jump relation reduces equation (2.21) to:

$$\dot{\rho}_m^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \sum_{l=1}^2 \int_{A_{l,i}} w(\vec{y} - \vec{x}) \Omega_{mi} \rho_{l,i} (u_{li,k} - v_{si,k}) n_k dA(\vec{y}) + C_{\rho_m}, \quad (2.31)$$

where C_{ρ_m} is the rate of accumulation of the m chemical specie at the liquid/gas interface. This accumulation may arise as a result of liquid phase chemical reactions. The variable Ω_{mi} accounts for the assumed chemical stoichiometry of the gas phase chemical reaction within the interfacial surface layer. Conservation

of mass requires that

$$\sum_{m=1}^{NSP} \Omega_{mi} = 1 .$$

Since the liquid phase is idealized as being composed of a collection of globules, equation (2.31) can be written as:

$$\dot{\rho}_m^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \sum_d \sum_{l=1}^2 \int_{A_{d,l}} w(\mathcal{Y}-\mathcal{X}) \Omega_{mi} \rho_{l,i} (u_{li,k} - v_{sl,k}) n_k dA(\mathcal{Y}) + C_{\rho_m} . \quad (2.32)$$

The continuous integral over the liquid/gas interface is thus replaced with a summation of integrals over each individual globule⁺⁺⁺ surface (A_d). An average globule density is defined by

$$\frac{4}{3} \pi r^3 \rho_d = \int_{V_d} \rho dV .$$

Taking the derivative of the above expression with respect to time gives

$$\frac{d}{dt} \left(\frac{4}{3} \pi r^3 \rho_d \right) = - \int_{A_d} \rho (u_{l,k} - v_{s,k}) n_k dA .$$

Putting this expression back into equation (2.32) and dividing all globules in a particular volume into classes and type result in

$$\dot{\rho}_m^S = C_{\rho_m} - \sum_{l=1}^2 \int F_l(\vec{\zeta}_p, \vec{x}_p, \eta) \Omega_{mi} \frac{d}{dt} \left(\frac{4}{3} \pi r_i^3 \rho_{d,i} \right) d\vec{\zeta}_i . \quad (2.33)$$

Momentum interface condition

Applying the liquid/gas interface jump relation for the momentum transfer

⁺⁺⁺ The nomenclature globule and drop is used interchangeably.

and neglecting the effects of surface tension gradients result in

$$\mathbf{F}^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \sum_{i=1}^2 \int_{A_{\gamma,i}} w(\mathbf{y}-\mathbf{x}) [\rho_{l,i} \mathbf{u}_{l,i} (\mathbf{u}_{l,i} - \mathbf{v}_{s,i}) + p_l \mathbf{I} - \boldsymbol{\tau}_l] \cdot \hat{\mathbf{n}} dA(\mathbf{y}) + \mathbf{C}_{p_g} \quad (2.34)$$

where $\mathbf{C}_{p_g}$ is the rate of momentum accumulation at the liquid/gas interface. This momentum accumulation may arise because of the formation of gaseous products from liquid phase chemical reactions. The liquid phase is composed of a collection of globules with an average globule velocity defined as

$$\frac{4}{3} \pi r^3 \rho_d \mathbf{v} = \int_{V_d} \rho_d \mathbf{u}_d dV.$$

Taking the derivative of this with respect to time results in

$$\frac{d}{dt} \left(\frac{4}{3} \pi r^3 \rho_d \mathbf{v} \right) = - \int_{A_d} [\rho_d \mathbf{u}_d (\mathbf{u}_d - \mathbf{v}_d) + p_d \mathbf{I} - \boldsymbol{\tau}_d] \cdot \hat{\mathbf{n}} dA.$$

Putting this expression back into equation (2.34) and dividing all of the globules in a specific volume during a certain occurrence into classes and type gives

$$\mathbf{F}^S = \mathbf{C}_{p_g} - \sum_{i=1}^2 \int \frac{d}{dt} \left(\frac{4}{3} \pi r_i^3 \rho_{d,i} \mathbf{v}_i \right) F_i(\boldsymbol{\zeta}, \mathbf{x}_p, \mathbf{t}) d\boldsymbol{\zeta}_i. \quad (2.35)$$

Internal energy interface condition

Neglecting viscous dissipation and work done by surface tension at the interface allows the jump condition to be manipulated thereby obtaining

$$\dot{Q}^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \sum_{i=1}^2 \int_{A_{\gamma,i}} w(\mathbf{y}-\mathbf{x}) [\rho_{l,i} \mathbf{e}_{l,i} (\mathbf{u}_{l,i} - \mathbf{v}_{s,i}) + \mathbf{q}_{l,i}] \cdot \hat{\mathbf{n}} dA(\mathbf{y}) + C_{p_g}, \quad (2.36)$$

where C_{p_g} is the rate of energy accumulation at the liquid/gas interface. The

average globule internal energy is defined as

$$\frac{4}{3}\pi r^3 \rho_d e_d = \int_{V_d} \rho_l e_l dV .$$

Taking the derivative of this with respect to time gives

$$\frac{d}{dt} \left(\frac{4}{3}\pi r^3 \rho_d e_d \right) = - \int_{A_d} [\rho_l e_l (\vec{u}_l - \vec{v}_d) + \vec{q}_l] \cdot \hat{n} dA + W_{stress} , \quad (2.37)$$

where the work done by the stresses is given by

$$W_{stress} = -\frac{1}{2}(\vec{v} - \vec{u})^2 \frac{d}{dt} \left(\frac{4}{3}\pi r^3 \rho_d \right) - \frac{4}{3}\pi r^3 \rho_d \frac{d\vec{v}}{dt} \cdot (\vec{v} - \vec{u}) .$$

Equation (2.37) is a particular statement of the first law of thermodynamics. Substituting this expression into equation (2.36) and dividing the globules into classes and type result in:

$$\dot{Q}^S = C_p - \sum_{i=1}^2 \int \left\{ \frac{d}{dt} \left[\left(\frac{4}{3}\pi r_i^3 \rho_{d,i} \right) (e_{d,i} + \frac{1}{2}[\vec{v}_i - \vec{u}]^2) \right] F(\vec{\zeta}_i, \vec{x}_i, \eta) d\vec{\zeta}_i \right\} . \quad (2.38)$$

KE interface condition

The mechanical energy jump relation allows the liquid/gas interfacial work interaction to be written as:

$$\dot{W}^S = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\gamma=1}^N \sum_{i=1}^2 \int_{A_{l,i}} w(\vec{y} - \vec{x}) \left[\rho_{l,i} \frac{\vec{u}_{l,i} \cdot \vec{u}_{l,i}}{2} (\vec{u}_{l,i} - \vec{v}_{s,i}) - (\vec{\tau}_{l,i} - \vec{p}_{l,i}) \right] \cdot \vec{u}_{l,i} \cdot \hat{n} dA(\vec{y}) + C_q , \quad (2.39)$$

where C_q is the rate of accumulation of kinetic energy at the liquid/gas interface. The average globule kinetic energy is defined as

$$\frac{4}{3}\pi r^3 \rho_d \frac{\vec{v} \cdot \vec{v}}{2} = \int_{V_d} \rho_l \frac{\vec{u}_l \cdot \vec{u}_l}{2} dV .$$

Differentiating this expression with respect to time and substituting back into equation (2.39) result in

$$\dot{W}^S = C_q - \vec{u} \cdot \vec{C}_{p_d} + \frac{\vec{u} \cdot \vec{u}}{2} \sum_m C_{p_m} - \sum_{i=1}^2 \int \frac{4}{3} \pi r_i^3 \rho_{d,i} \frac{d\vec{v}_i}{dt} \cdot \vec{u}'' F(\vec{\zeta}_i, \vec{x}_i, t) d\vec{\zeta}_i . \quad (2.40)$$

This shows explicitly the interaction of a globule with the turbulent velocity fluctuation.

The following section formulates the sub-models needed in order to evaluate the source terms in both the averaged gas phase equations and the liquid globule number conservation equations (eq. (2.7) and (2.8)). These source terms depend upon the evolution of the globule state variables and the local gas environment.

3 SUB-MODEL FORMULATIONS

3.1 Turbulence Closure

Various models have been proposed to achieve closure of the system of equations for a turbulent reacting flow. The k - ϵ two-equation model of Jones and Launder³³ is adopted. It is assumed that the Reynolds stress and the rate of strain exhibit a linear relationship as follows:

$$\widetilde{\bar{\rho} u_i'' u_j''} = \frac{2}{3} \delta_{ij} (\bar{\rho} k + \mu_t \frac{\partial \tilde{u}_k}{\partial x_k}) - \mu_t (\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}) . \quad (3.1)$$

A gradient-diffusion model is employed for turbulent flux of scalar quantities, namely

$$\widetilde{\bar{\rho} u_j'' \psi''} = - \frac{\mu_t}{\sigma_t} \frac{\partial \tilde{\psi}}{\partial x_j} , \quad (3.2)$$

where σ_t is the turbulent Prandtl/Schmidt number for ψ . The turbulent viscosity is given by

$$\mu_t = C_\mu \bar{\rho} \frac{k^2}{\epsilon} , \quad (3.4)$$

with the turbulence constant $C_\mu = 0.09$. The turbulence kinetic energy k is defined as

$$k \equiv \tilde{q}'' = \frac{\widetilde{u_i'' u_i''}}{2} ,$$

and the dissipation rate of turbulence kinetic energy is given by

$$\overline{\epsilon} = \overline{u_i'' \frac{\partial \tau_{ik}''}{\partial x_k}} .$$

Under the present circumstances, equation (2.28) becomes^{*}

$$\frac{\partial \rho k}{\partial t} + \vec{\nabla} \cdot [\rho k \vec{u} - \frac{\mu}{Pr_k} \vec{\nabla} k] = -\frac{2}{3} \rho k \vec{\nabla} \cdot \vec{u} - \rho \epsilon + \vec{\tau} : \vec{\nabla} \vec{u} + \dot{W}^S , \quad (3.5)$$

where Pr_k is the turbulent Prandtl number for k . A transport equation for the dissipation rate of turbulence kinetic energy²⁹ is given by:

$$\begin{aligned} \frac{\partial \rho \epsilon}{\partial t} + \vec{\nabla} \cdot [\rho \epsilon \vec{u} - \frac{\mu}{Pr_\epsilon} \vec{\nabla} \epsilon] = & -(\frac{2}{3} C_{\epsilon_1} - C_{\epsilon_3}) \rho \epsilon \vec{\nabla} \cdot \vec{u} + \\ & \frac{\epsilon}{k} [C_{\epsilon_1} \vec{\tau} : \vec{\nabla} \vec{u} - C_{\epsilon_2} \rho \epsilon + C_s \dot{W}^S] . \end{aligned} \quad (3.6)$$

The following sets of constants are recommended:

$$\begin{aligned} C_{\epsilon_1} &= 1.44 & C_{\epsilon_2} &= 1.92 & C_{\epsilon_3} &= -1.0 \\ Pr_k &= 1.0 & Pr_\epsilon &= 1.3 & C_s &= 1.50 . \end{aligned}$$

It is important to point out that the above gradient-diffusion model neglects the effects of counter-gradient diffusion, that is, turbulent diffusion of a species against its mean gradient. The available literature gives no concrete evidence of significant effects of counter-gradient diffusion in practical systems.

With this turbulence model, the averaged gas phase equations for a chemically reactive turbulent mixture of ideal gases with imbedded condensed

* The averaging notation is now suspended with all variables understood to be averaged variables where appropriate.

liquid phases are summarized below:

species continuity

$$\frac{\partial \rho Y_m}{\partial t} + \vec{\nabla} \cdot [\rho Y_m \vec{u} - \rho D \vec{\nabla} Y_m] = \dot{\rho}_m^c + \dot{\rho}_m^s \quad (3.7)$$

momentum

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot [\rho \vec{u} \vec{u} + (p + \frac{2}{3} \rho k) \vec{I} - \vec{\tau}] = \vec{F}^s \quad (3.8)$$

internal energy

$$\frac{\partial \rho e}{\partial t} + \vec{\nabla} \cdot [\rho e \vec{u} + \vec{q}] = -p \vec{\nabla} \cdot \vec{u} + \rho \dot{e} + \dot{Q}^c + \dot{Q}^s \quad (3.9)$$

state relations

$$p = \rho R_u T \sum_{m=1}^{NSP} \left(\frac{Y_m}{\hat{W}_m} \right) ; e = \sum_{m=1}^{NSP} Y_m e_m(T) ; h_m(T) = e_m(T) + R_u T \quad (3.10)$$

transport coefficients

$$\mu = \mu_{laminar} + \mu_t ; \lambda = \frac{\mu c_p}{Pr} ; \rho D = \frac{\mu}{Sc} . \quad (3.11)$$

This completes the gas phase formulation. The gas phase chemistry, the collision, breakup, and the evolution of the liquid globule state variables are modelled in what follows.

3.2 Gas Phase Chemistry

Gas phase combustion modelling depends upon the problem at hand. In

combusting flow CFD, computer time and storage constraints place severe restrictions on the complexity of the reaction mechanisms that can be incorporated. Moreover, detailed reaction chemistry is rarely available for practical bipropellant systems. Accordingly, multidimensional spray combustion calculations have used highly simplified chemical kinetic schemes, with one or at most few reactions, to represent the combustion process.

Rocket engine combustion flames are typically of the premixed type. Hence, the approximation of local chemical equilibrium is not appropriate. A popular approach in spray combustion modelling involves application of Spalding's³⁴ eddy-breakup model for turbulent reaction. This approach assumes that the mean reaction rate is determined solely by the scale reduction via a process of turbulent vortex stretching. There is no explicit accounting of chemical kinetics and the rate of combustion is entirely turbulent mixing-controlled. Application of the eddy-breakup model requires the evaluation of the instantaneous species mass fractions which are not readily available. To circumvent this problem, Magnussen and Hjertager³⁵ proposed a related method which only requires the evaluation of averaged species mass fractions. For the pre-ignition period, chemical kinetics are important. The chemical time, characterizing the prereactions leading to autoignition, is large in comparison to the turbulent mixing time. It is thus legitimate to replace the instantaneous variables in the equation for reaction rates by their averaged values.

The chemical reactions are symbolized by

$$\sum_{m=1}^{NSP} v'_{m,r} M_m \rightarrow \sum_{m=1}^{NSP} v''_{m,r} M_m$$

where M_m represents one mole of species m and $v'_{m,r}$ and $v''_{m,r}$ are integral stoichiometric coefficients for reaction r . Kinetic reactions proceed at a rate given by the law of mass action:

$$\dot{\omega}_{kin} = k_f \prod \left(\frac{\rho_m}{\hat{W}_m} \right)^{v'_{m,r}} - k_b \prod \left(\frac{\rho_m}{\hat{W}_m} \right)^{v''_{m,r}}. \quad (3.12)$$

The coefficients k_f and k_b are assumed to be of a generalized Arrhenius form:

$$k_f = A_f T^{\zeta_f} \exp\left(-\frac{E_f}{T}\right)$$

$$k_b = A_b T^{\zeta_b} \exp\left(-\frac{E_b}{T}\right)$$

where E_f and E_b are activation temperatures, and A_f , A_b , ζ_f , ζ_b are constants for a particular reaction.

The model of Magnussen and Hjertager³⁵ assumes a one-step global chemistry such as:



where σ is the stoichiometric ratio of mass of oxidizer to that of fuel. The ratio $\frac{k}{e}$ is an eddy-breakup time scale. Consequently, the mixing limited reaction rate is given by

$$\dot{\omega}_{mix} = A_1 \frac{e}{K} \min\left(C_F, \frac{C_O}{\sigma}\right) \quad (3.13)$$

where A_1 is a model constant with C_F and C_O being respectively the fuel and

oxidizer molar concentrations. The actual reaction rate is taken to be

$$\dot{\omega} = \min(\dot{\omega}_{mix}, \dot{\omega}_{kin}) .$$

This procedure is not directly applicable to multi-step reactions. Heuristic arguments must be invoked when an extension to multi-step reactions is desired.

With the reaction rate determined, the chemical source term in the species continuity equation is given by

$$\dot{\rho}_m^c = \hat{W}_m \sum_r (v_{m,r}'' - v_{m,r}') \dot{\omega}_r , \quad (3.14)$$

and the chemical heat release term in the energy equation is given by

$$\dot{Q}^c = \sum_r Q_r \dot{\omega}_r , \quad (3.15)$$

where Q_r is the heat of combustion at a reference temperature,

$$Q_r = \sum_m (v_{m,r}' - v_{m,r}'') (\Delta h_f^0)_m , \quad (3.16)$$

and $(\Delta h_f^0)_m$ is the heat of formation of species m at the reference temperature. Specific reactions for a particular problem will be discussed later when applications are illustrated.

3.3 Globule Collisions

Two types of collisions are considered. The first type involves the impingement of two unlike continuous liquid streams and the second concerns the coalescence or scattering among like globules in the dispersed liquid cluster.

Collisions between two unlike globules in the dispersed liquid cluster are not considered. It is argued that the resultant spray after impingement will have a nearly uniform velocity thereby making the probability of collision between two unlike liquid droplets small.

Similar to the procedure employed in kinetic theory under the assumptions of binary collisions only, a mathematical formulation for the collision source term may be derived. It is convenient to decompose the collision source (eq. 2.3) term into:

$$\dot{F}_{coll} = \Gamma^{(+)} - \Gamma^{(-)} , \quad (3.17)$$

where $\Gamma^{(+)}$ represents the collision production and $\Gamma^{(-)}$ accounts for collisional destruction. For a collision at a given position between two globules with known approach attributes, the attributes and number of outgoing globules are in principle completely determined by the local averaged gas properties, the liquid material properties, and the geometry of the collision. Since all collisions cause the incident globules to change their range of attributes, the number of globules scattered out of the range during an infinitesimal time interval must be of the form:

$$\Gamma^{(-)} d\vec{S} dt = F(\vec{S}, t) d\vec{S} . \quad \text{(number of collisions at time } dt \text{)} . \quad (3.18)$$

This relation states that the number of globules scattered out of the range equals the number of globules in the range multiplied by the total number of collisions which these globules experience in time dt . An expression for the total number of globules added to the range is

$$\Gamma^{(+)} dS dt = \Psi(S', t) dS' \cdot \text{(total number of collisions at time } dt), \quad (3.19)$$

where Ψ gives the globule number distribution produced in a collision and S' refers to the resultant attributes. Some physical modelling is required in order to describe the outcome of a collision which occurs on a "sub-scale" level. The number of collisions during a certain time interval is influenced by the interactions of the flow fields near the globules. This interaction will be indirectly included in the description of the globule collision geometry. Knowing the collision geometry, the number of collisions during a certain time interval can be expressed in terms of the approach attributes of the two globule species.

The two types of collisions are each treated separately. Impingement among the two immiscible intact liquid cores is fundamentally different from the coalescence or scattering among drops in the dispersed liquid clusters. The collision geometry in an impingement collision is more-or-less deterministic whereas that of a natural coalescence or scattering among drops in the dispersed clusters is stochastic.

Liquid stream impingement

Consider two cylindrical jets colliding obliquely, it is found⁹ that the liquids spread into a flat sheet flowing in a plane perpendicular to that containing the axes of the two jets. Clayton³⁶ stated without proof that depending upon the relative dynamic pressures of the two streams several differing flow fields will result downstream of impingement. For example, at a dynamic pressure ratio of one, a double stagnation point will occur at the impingement point, and for jet dynamic pressures which are unequal, the stream having the lower stagnation

pressure will stagnate against the other stream (Fig. 3). The present formulation represents a continuous liquid stream by a collection of discrete globules. Therefore, observations of impinging jets must be extended to discrete globules under the assumption that the liquid jet is the limiting case of a highly dense collection of globules.

The steps involved in the impingement collision of two immiscible globules are postulated to be:

- (1) period of deformation, where large globule surface oscillations along with a certain amount of deviation from sphericity are induced;
- (2) period of restitution, where mutual surface interactions occur.

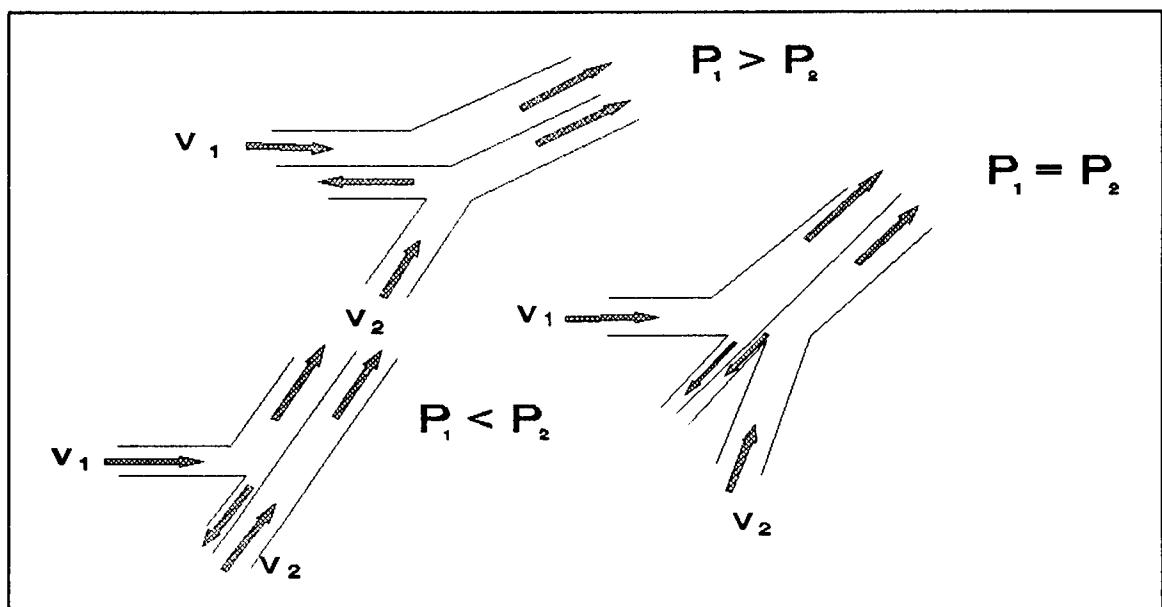


Figure 3. Schematic representations of the impingement region for unlike impinging free liquid jets. P is dynamic pressure (Ref. 36).

A possible mutual surface interaction is the interfacial surface chemical reaction which is inherent in hypergolic bipropellant systems. That is, when two

hypergolic globules come in contact, a chemical reaction may occur along the contact surface thereby releasing heat and generating gaseous products. The binary globule collision geometry is illustrated in Figure 4. Given the velocity

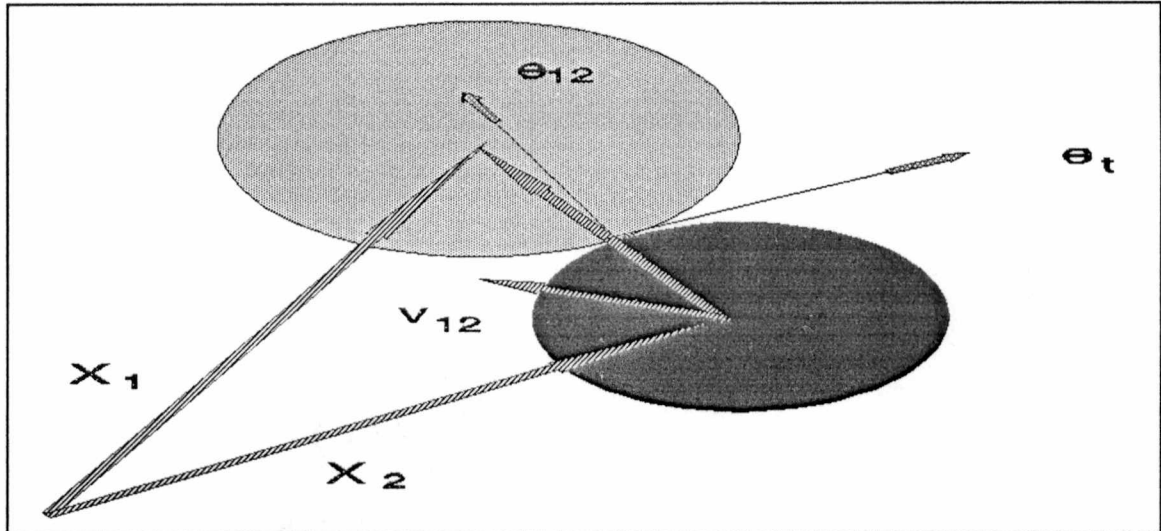


Figure 4. Schematic representation of binary globule collision geometry.

vectors $\vec{v}_i$ and $\vec{v}_k$ of two globules of species i and k , a unit vector in the plane perpendicular to that containing the velocity axes of the two globules is given by

$$\hat{e}_t = \frac{m_i \vec{v}_i + m_k \vec{v}_k}{|m_i \vec{v}_i + m_k \vec{v}_k|} \quad (3.20)$$

where $m = \frac{4}{3} \pi \rho_d r^3$ is the mass of a globule. It is assumed that for a binary liquid globule pair, a unit vector along the plane of impact is given by

$$\hat{e}_{ik} = \frac{\vec{v}_k \times \vec{v}_i}{|\vec{v}_k \times \vec{v}_i|} \times \hat{e}_t. \quad (3.21)$$

This assumption is based upon intuitive notions about how liquid surfaces interact. Equation (3.21) can be viewed as indirectly accounting for the effects of the interactions of the flow fields about the binary globule pair. Collision is impending if and only if:

$$|\vec{x}_i - \vec{x}_k| \leq r_i + r_k ; \vec{v}_{ki} \cdot \hat{e}_{ik} > 0 \quad (3.22)$$

where $\vec{v}_{ki} = \vec{v}_k - \vec{v}_i$ is the approach relative velocity between the binary globule pair.

Assuming that binary globule collisions are similar to those among hard spheres, the collision source term for the intact liquid core (eq. 2.7) may be written as:

$$\begin{aligned} \dot{g}_{coll,i} = \sum_{k=i,k} [& \int \Psi_{ik}(\vec{\zeta}'_i; \vec{\zeta}'_k, \vec{x}, \eta) g_i(\vec{\zeta}'_i, \vec{x}_i, \eta) g_k(\vec{\zeta}'_k, \vec{x}_k, \eta) \pi(r_i + r_k)^2 (\vec{v}_{ki} \cdot \hat{e}_{ik}) d\vec{\zeta}'_k d\vec{\zeta}'_i - \\ & \int g_i(\vec{\zeta}_i, \vec{x}_i, \eta) g_k(\vec{\zeta}_k, \vec{x}_k, \eta) \pi(r_i + r_k)^2 (\vec{v}_{ki} \cdot \hat{e}_{ik}) d\vec{\zeta}_k] \end{aligned} \quad (3.23)$$

Equation (3.23) is a direct mathematical statement of the balance between production (eq. 3.19) and destruction (eq. 3.18) of the number of globules during an impingement collision.

Considering the two globules as a single system, it is noted that there is no net impulsive, external force. Thus, the total momentum of the globule pair is conserved. Consequently, the values of the globules' velocities after collision are given in terms of their values before the collision by

$$\vec{v}'_i = \vec{v}_i + M_{ki}(\vec{v}_{ki} - \vec{v}'_{ki}) , \quad (3.24)$$

where $M_{ki} = \frac{m_k}{m_k + m_i}$. The resultant relative velocity after collision is assumed to be of the form

$$\vec{v}'_{ki} = \eta_{ki}(\vec{v}_{ki} \cdot \hat{e}_i) \hat{e}_i - \epsilon_{ki}(\vec{v}_{ki} \cdot \hat{e}_{ik}) \hat{e}_{ik} \quad (3.25)$$

where the coefficient of restitution ϵ_{ki} depends upon the propellant material

properties and is related to the dissipation of energy at the binary globule interface. An expression for the coefficient of restitution may be written as

$$\epsilon_{ki} = \frac{R}{P},$$

where R and P are respectively restitution and deformation forces along the line of impact. The deformation impulse along the line of impact can be shown to be

$$P \Delta t_{def} = m_k M_{ik} \bar{v}_{ki} \cdot \hat{e}_{ik} \quad (3.26)$$

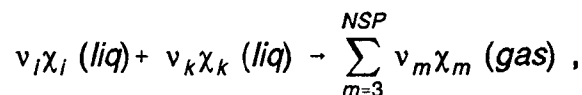
and the component of restitution force along the line of impact depends upon the details of the interfacial interactions. Non-reactive impinging liquid jet experiments suggest a value on the order of zero for ϵ_{ki} . This implies a negligible period of restitution with the final velocities being virtually the same for the two globules. For the case of reactive bipropellant streams, the coefficient of restitution is assumed to be of the form

$$\epsilon_{ki} = \epsilon_{ki}^0 + \epsilon_{ki}^c$$

where ϵ_{ki}^0 is an intrinsic coefficient of restitution of the bipropellant system and ϵ_{ki}^c is a coefficient of restitution generated by interfacial chemical reactions. For most bipropellant systems, it is observed that $\epsilon_{ki}^0 \ll 1$. An estimate of the restitution generated by interfacial reactions can be obtained if the amount of heat released during the reaction is related to an equivalent mechanical work.

Heterogeneous chemical reaction along a material interface is not well understood. Somogyi and Feiler³⁷ determined the heat release rates produced by the reactions of hydrazine with nitric acid in a bomb calorimeter under conditions of forced mixing. The heat release rate was shown to vary with

injection velocity. The increase in heat release rate with injection velocity was attributed to an increase in interfacial area. Assuming a one-step liquid phase chemical reaction such as:



the law of mass action may be invoked to obtain the reaction rate in the form

$$K_{ik} = -v_i B f_{mix,ik} \exp\left(-\frac{E_a}{T_i}\right) \int \frac{m_k}{\dot{W}_k} g_k(\vec{\zeta}_k, \mathbf{x}_k, \eta) d\vec{\zeta}_k , \quad (3.27)$$

where the mass average liquid mixture temperature is

$$T_i = \frac{m_i T_{d,i} + m_k T_{d,k}}{m_i + m_k} .$$

The constants B and E_a need to be determined for the particular bipropellant system and the fractional mixing ratio, $f_{mix,ik}$ is assumed to be of the form

$$f_{mix,ik} \equiv \frac{\text{mixing volume}}{\text{volume available}} = \int \pi (r_i + r_k)^2 (\vec{v}_{ki} \cdot \hat{\mathbf{e}}_{ik}) g_k(\vec{\zeta}_k, \mathbf{x}_k, \eta) dt d\vec{\zeta}_i . \quad (3.28)$$

An expression for the globule number collision production is postulated to be

$$\Psi_{ik}(\vec{\zeta}'_i, \vec{\zeta}'_k, \mathbf{x}, \eta) = \frac{1}{2} \{ \delta(\vec{\zeta}_i - \vec{\zeta}'_i) \exp(-\int K_{ik} d\eta) + \delta(\vec{\zeta}_k - \vec{\zeta}'_k) \exp(-\int K_{ki} d\eta) \} . \quad (3.29)$$

This expression states that when two unlike globules collide, one or less globule of each kind is produced with attributes $\vec{\zeta}'$. The amount of heat released during the reaction is estimated from the data of Somogyi and Feiler. A maximum heat release rate per mass of oxidizer consumed, $\mathfrak{R}_{\max}$ is given³⁷ for perfectly mixed hypergolic bipropellant systems. Employing this data, the heat released is

$$Q_I = \Delta m_{ox} \mathfrak{R}_{\max} \Delta t_{mix}$$

where Δm_{ox} is the mass of oxidizer consumed and the mixing time interval is obtained from

$$\Delta t_{mix} = \int \frac{1}{f_{mix,ik}} dt .$$

This amount of heat will be used to raise the temperature of the gaseous products released during the reaction. The mass of propellant consumed is given by

$$\Delta m_i = \int g(\zeta_p, x_p, \eta) m_i [\exp(\int K_{ik} d\eta) - 1] dS_i .$$

Application of the first law of thermodynamics leads to

$$\Delta m_g C_{p_g} \Delta T_g = Q_I ,$$

where Δm_g is the total mass of gaseous products released during the reaction and ΔT_g is the temperature rise of the product gases generated at the interface. An equivalent pressure rise is obtained as follows:

$$\Delta p = \rho_g R_g \Delta T_g .$$

This pressure rise is transformed into a force along the direction of impact by assuming the following expression for the collisional surface contact radius:

$$r_{contact} = \frac{We^{.2}}{2 + We^{.2}} \sqrt{r_i r_k} ,$$

where We is a Weber number for the binary globule pair. This Weber number is given by

$$We = \sqrt{\frac{\rho_i \rho_k r_i r_k}{\sigma_i \sigma_k}} (\nabla_{ki} \cdot \hat{e}_{ik})^2 ,$$

where σ is the liquid surface tension. The expression assumed for the contact radius is analogous to what is given by Herz³⁸ for impact between two elastic bodies. Hence, the restitution force due to interfacial reaction is

$$R = \Delta p \pi r_{contact}^2$$

and the coefficient of restitution due to surface reactions is

$$\epsilon_{kl}^c = \frac{B_e R \Delta t_{mix}}{P \Delta t_{def}} , \quad (3.30)$$

where B_e is a model constant on the order of 0.5 . For lack of better data, the coefficient η_{kl} is assumed to be

$$\eta_{kl} = \sqrt{\epsilon_{kl}} .$$

The resultant attributes of globules produced during a collision are

$$\vec{\zeta}_i' = \begin{Bmatrix} r_i' \\ \nabla_i' \\ y_i' \\ \dot{y}_i' \\ T_{d,i} \\ \theta_i \end{Bmatrix}$$

where the assumption is being made that the size and temperature of a globule do not change during a collision. Keeping the globule temperature constant is justified by the restriction that for an immiscible fluid mixture the temperature of each constituent is determined by the constitutive variables of that constituent

alone. The collision induced deformation y'_i and oscillation $\dot{y}'_i$ will be addressed in the atomization/breakup model.

Expressions for the rate of accumulation of mass, momentum, and energy at the globule/gas interfaces are obtained in such a way that mass, momentum, and energy are conserved during a collision resulting in a liquid phase reaction. Suitable forms for these expressions are:

$$C_{\rho_m} = - \int \frac{m_i}{\hat{W}_i} v_m \hat{W}_m K_{ik} g(\vec{\zeta}_i, \vec{x}_i, t) d\vec{\zeta}_i dt, \quad (3.31 a)$$

$$\begin{aligned} C_{\rho_a} &= \bar{v}_l \sum_m C_{\rho_m}, \\ C_{\rho_e} &= -Q_l, \end{aligned} \quad (3.31 b)$$

where $\bar{v}_l$ is the mass average mixture velocity of the binary globule pair along the binary globule interface and is given by

$$\bar{v}_l = \frac{m_i \bar{v}_i + m_k \bar{v}_k}{m_i + m_k}.$$

The rate of kinetic energy accumulation at the interface is assumed to be negligible.

Collisions among like globules making up the intact liquid cores are assumed to result in the production of a coalesce pair. The state variables for the coalesce pair are obtained by simple arithmetic averaging. A justification for this assumption is due to the continuity of the intact liquid core. Continuity dictates that two like globules belonging to the intact liquid core must have the same state vectors if they are at the same spatial location.

Dispersed liquid coalescence and scattering collisions

The drop collision and coalescence model of O'Rourke²⁰ is used to simulate the collision and coalescence among drops in the dispersed liquid clusters. As previously mentioned, collisions among unlike drops making up the dispersed liquid clusters are not considered. According to O'Rourke, the dispersed liquid collision source term (eq. 2.8) can be written as

$$\dot{f}_{coll,i} = \int \Phi(\vec{\zeta}'_{i,1}, \vec{\zeta}'_{i,2}, \vec{x}_p) f(\vec{\zeta}'_{i,1}, \vec{x}_p) f(\vec{\zeta}'_{i,2}, \vec{x}_p) \pi(r_{i,1} + r_{i,2})^2 |\vec{v}_{i,1} - \vec{v}_{i,2}| d\vec{\zeta}_{i,1} d\vec{\zeta}_{i,2} \quad (3.32)$$
$$- f(\vec{\zeta}_{i,1}, \vec{x}_p) \int \pi(r_{i,1} + r_{i,2})^2 |\vec{v}_{i,1} - \vec{v}_{i,2}| f(\vec{\zeta}_{i,2}, \vec{x}_p) d\vec{\zeta}_{i,2} .$$

Collisions among droplets in the dispersed liquid clusters are stochastic in nature and Φ is interpreted as a collision probability function defined so that $\Phi d\vec{\zeta}_i$ is the probable number of drops per unit spatial volume with properties in the implied intervals that result from a collision between a droplet with subscript 1 attributes and one with subscript 2 attributes.

The outcome of the collision is either a grazing collision (in a grazing collision the colliding drops maintain their sizes and temperatures but undergo velocity changes²⁰) or it is coalescence depending on whether the collision impact parameter, is greater or less than a critical value. Coalescence is the likely result of all dispersed cluster collisions except those that involve nearly equal-sized drops traveling at high velocities relative to each other. Details of the computations may be obtained by consulting Ref. 20.

3.4 Globule Breakup

Consider the impingement of two liquid streams. Thereupon impingement,

a sheet is formed. If the liquids are immiscible, an interface is created partitioning the sheet into upper and lower layers. The sheet is idealized as being composed of a collection of quasi-spherical globules interacting across a material interface. These globules will eventually breakup to form a droplet spray. It should be noted that details of the sheet structure (i.e., thickness and flux variations) are not well represented by the globule train idealization. Nevertheless, a reasonable simulation of the gross effects of the atomization process should be possible.

The cause of instabilities leading to sheet breakup is due to amplification of disturbances generated by the injection mechanism, the impingement hydrodynamic impact forces, and the interaction of the sheet with the surrounding gas. When the waves generated by these disturbances reach a critical amplitude, fragments of the sheet are torn off. The fragments contract into ligaments and finally break down into drops.

Similar to Reitz¹² and Hinze³⁹ an atomization model is formulated based upon the assumption that the dynamics and breakup of a liquid sheet are indistinguishable from those of a train of globules with equal diameters. The TAB (Taylor Analogy Breakup) model of O'Rourke and Amsden¹³ is extended for the breakup of liquid columns formed by impinging jets. This model is based on an analogy between an oscillating and distorting globule and a spring-mass system. The restoring force of the spring is analogous to the surface tension forces. The external force on the mass is analogous to the superposition of the globule hydrodynamic impact force and the gas aerodynamic force. To this analogy is added the damping forces due to liquid viscosity. According to Ref. 13, the major limitation of the TAB model is that only one oscillation mode can be tracked, and

in reality there are many such modes. Only the fundamental mode is tracked. This is the longest-lived and, therefore, the most important mode of oscillation, but for large applied external forces, other modes are certainly excited and contribute to globule breakup. Despite this limitation, good agreement between experimentally observed and predicted breakup times have been reported.

The equation of a damped, forced harmonic oscillator is

$$m\ddot{x} + d\dot{x} + kx = F, \quad (3.33)$$

where x is the displacement of the equator of the globule from its equilibrium position. The applied force F consists of a superposition of aerodynamic and impulsive impact forces and is written as

$$F = \begin{cases} F_{imp} & t < \Delta t_{def} \\ F_{aero} & t \geq \Delta t_{def} \end{cases}.$$

In accordance with the Taylor analogy, the physical dependencies of the coefficients in equation (3.33) are

$$\begin{aligned} \frac{F}{m} &= \begin{cases} C_{F_1} \frac{\rho u^2}{\rho_l r} & t \geq \Delta t_{def} \\ C_{F_2} \frac{P}{m} & t < \Delta t_{def} \end{cases}, \\ \frac{k}{m} &= C_k \frac{\sigma}{\rho_l r^3}, \\ \frac{d}{m} &= C_d \frac{\mu_l}{\rho_l r^2}, \end{aligned} \quad (3.34)$$

where u is the relative velocity between the gas and the globule, P is the deformation force (eq. 3.26), and σ is the gas-liquid surface tension coefficient. Equation (3.33) is nondimensionalized by letting $y = \frac{x}{C_b r}$ where C_b is a constant

to be determined. The resulting analogy for the displacement of the equator of a globule from its equilibrium spherical position is

$$\ddot{y} + \frac{2}{t_d} \dot{y} + \omega_n^2 y = \frac{F}{m C_b r} , \quad (3.35)$$

where the globule natural frequency ω_n and the damping time constant t_d are given by

$$\begin{aligned} \omega_n^2 &= \frac{C_k \sigma}{\rho_l r^3} , \\ \frac{1}{t_d} &= \frac{C_d \mu_l}{2 \rho_l r^3} . \end{aligned} \quad (3.36)$$

Breakup is assumed to occur if and only if $y > 1$.

Consider the time period during which the impulsive force is dominant (i.e., $t \leq \Delta t_{def}$) and assuming negligible effects of liquid viscosity, the TAB analogy for the globule reduces to:

$$\ddot{y} + \omega_n^2 y = C_{F_2} \frac{P}{m C_b r} . \quad (3.37)$$

The solution to this equation assuming constant coefficients is

$$y(t) = C_{F_2} \frac{P}{m \omega_n^2 C_b r} + \left[y_0 - C_{F_2} \frac{P}{m \omega_n^2 C_b r} \right] \cos \omega_n t + \frac{\dot{y}_0}{\omega_n} \sin \omega_n t \quad (3.38)$$

where y_0 and $\dot{y}_0$ are initial conditions produced by the injection mechanism. Assuming that $\omega_n \Delta t_{def} \ll 1$, the solution reduces to

$$\begin{aligned} y'(\dot{t}) &= y_0 \\ \dot{y}'(\dot{t}) &= \dot{y}_0 + C_{F_2} \frac{P \Delta t_{def}}{m C_b r} \end{aligned} \quad (3.39)$$

where the prime indicates that these are also the resultant attributes after an impingement collision.

For the time period greater than the duration of the impulse (i.e., $t > \Delta t_{def}$), the solution is:

$$\begin{aligned} y(\dot{t}) &= \frac{C_{F_1}}{C_k C_b} We + \exp\left(-\frac{t}{t_d}\right) \left[\left(y' - \frac{C_{F_1}}{C_k C_b} \right) \cos \omega t + \right. \\ &\quad \left. \frac{1}{\omega} \left(\dot{y}' + \frac{C_{F_1}}{C_k C_b} \frac{We}{t_d} \right) \sin \omega t \right], \end{aligned} \quad (3.40)$$

where

$$\begin{aligned} We &= \frac{\rho U^2 r}{\sigma}, \\ \omega^2 &= \omega_n^2 - \frac{1}{t_d^2}. \end{aligned} \quad (3.41)$$

The dimensionless constants are determined by matching with available data. O'Rourke and Amsden¹³ suggested the following values

$$C_k = 8, \quad C_d = 5, \quad C_{F_1} = \frac{1}{3}, \quad C_b = \frac{1}{2}.$$

According to Dombrowski and Hooper⁸, there is a critical impingement Weber number ($We_{imp,crit} = \frac{r \rho_i V_{ki}^2}{\sigma} > 132$) below which hydrodynamic impact waves will not significantly contribute to the breakup process. Acknowledging this critical

Weber number dependence and using the data of Heidmann et al.⁹, the constant C_{F_2} is estimated to be on the order of 0.3 .

The TAB model also predicts a velocity of the product drops normal to the path of the parent globule. At the time of breakup, the equator of the globule is traveling outward with velocity $\dot{x} = C_v C_b r \dot{\gamma}$. It seems reasonable that the product drops will have normal velocity

$$v_{\perp} = C_v C_b r \dot{\gamma} , \quad (3.42)$$

where C_v is a model constant depending upon the injection mechanism. Numerical experiments with plain orifice injectors have shown C_v to be approximately unity. Thus the spray angle is

$$\tan \frac{\theta_{cone}}{2} = \frac{v_{\perp}}{u} . \quad (3.43)$$

To predict the product drop sizes after breakup, the Sauter mean radius¹⁷ (SMR) of the size distribution of the product drops is assumed to be of the form:

$$\frac{r}{r_{32}} = D_0 + D_1 \left(\frac{\dot{\gamma}}{\omega_n} \right)^n \quad (3.44)$$

where D_0 , D_1 , and n are constants to be determined. This assumption is motivated by energy conservation arguments¹³ and dimensional analysis. The constants are determined by matching with available correlations¹¹ and the most suitable set thus far is found to be

$$D_0 = \frac{7}{3}, \quad D_1 = 3.0, \quad n = \frac{1}{2}.$$

For the distribution of sizes of the product drops, a quarter cosine wave raised to a power is used. The cumulative mass weighted size distribution function is taken to be

$$G(r) = 1 - \cos^a \left[\frac{\pi \frac{r}{\bar{r}}}{2 \left(\frac{r}{\bar{r}} \right)_{\max}} \right] \quad (3.45)$$

where a is an input constant and $\left(\frac{r}{\bar{r}} \right)_{\max}$ is a limit size normalized by the mass median size $\bar{r}$. This distribution function can be made to approximate many of the classical types such as Rosin-Rammler and chi-squared.

This atomization/breakup model is applicable to either the intact liquid core or the dispersed liquid cluster. A mathematical description of the breakup source term follows. Before doing so, it is convenient to decompose this source term into

$$\dot{F}_{bu} = \Lambda^{(+)} - \Lambda^{(-)} \quad (3.46)$$

where $\Lambda^{(+)}$ represents the breakup production and $\Lambda^{(-)}$ accounts for breakup destruction. A globule is broken up abruptly when the distortion parameter y exceeds unity. The number of globules undergoing breakup must be of the form:

$$\Lambda^{(-)} dS dt = F(x, \bar{v}, r, T_a, 1, \dot{y}, \theta, \eta) dx d\bar{v} dr dT_a d\dot{y} d\theta d\eta dt. \quad (3.47)$$

This expression states that the number of globules in a given range undergoing breakup in a certain time interval is equal to the number of globules with globule

surface distortion y exceeding unity multiply by the local flux of drops through the surface $y=1$. An expression for the total number of drops added to the range is

$$\Lambda^{(+)} d\vec{S} dt = B(\vec{S}', \hat{n}) d\vec{S} F(\vec{x}, \vec{v}, r, T_d, 1, \dot{y}, \theta, \hat{n}) d\vec{x} d\vec{v} dr dT_d d\dot{y} d\theta d\hat{n} \dot{y} dt, \quad (3.48)$$

where $B(\vec{S}', \hat{n})$ gives the drop number distribution produced during breakup with attributes $\vec{S}'$. The distribution function B is assumed to have the following form²⁹:

$$B = \frac{dG(\hat{n})}{d\hat{n}} \delta(T_d - T_d') \delta(y) \delta(\dot{y}) \delta(\theta) \frac{1}{2\pi} \int \delta[\vec{v} - (\vec{v}' + V_{\perp} \hat{n})] d\hat{n}, \quad (3.49)$$

where the integral is over normal directions to the relative velocity vector between the gas and a globule. The values of T_d' and $\vec{v}'$ are those of the parent globule just before breakup. A product drop is given the same temperature as the parent globule and its deformation and oscillation parameters are set to zero.

After breakup, a globule initially belonging to the intact liquid core generates product drops comprising the dispersed liquid cluster. Thus, using equations (3.46), (3.47), and (3.48), the breakup source term for the intact liquid core may be written as

$$\dot{g}_{bu,i} = \int g_i(\vec{x}_p, \vec{v}_p, r_p, T_{d,i}, 1, \dot{y}_i, \theta_i, \hat{n}_i) \dot{y}_i B(\vec{S}_p, \hat{n}) d\vec{v}_i dr dT_{d,i} d\dot{y}_i d\theta_i d\hat{n}_i - g_i(\vec{x}_p, \vec{v}_p, r_p, T_{d,i}, 1, \dot{y}_p, \theta_p, \hat{n}_p) \dot{y}_p. \quad (3.50)$$

The following relation is implied in the above expression

$$g(\theta=0) \equiv f(\theta=0) .$$

Similar expressions may be written for the dispersed liquid cluster under the stipulation that drops making up the dispersed liquid cluster breakup into smaller drops belonging to the dispersed liquid cluster.

3.5 Droplet Combustion

In order to determine the interphase energy and mass transfers, a spray combustion model must be constructed. This model needs to provide a reasonable estimate of the local propellant gasification rates without severely affecting the computational efficiency of the CFD code. For the present work, a bipropellant envelope flame model¹⁷ is adopted. With this model, an oxidizer droplet present in a fuel vapor rich environment is capable of combusting with an envelope flame in much the same way as a fuel droplet burning in an oxidizer environment. The primary assumptions are:

(a) The heat and mass transfer of a drop are not significantly influenced by the presence of other drops.

(b) The overall heat and mass transfer processes are spherically symmetric with convection accounted for by using a multiplicative correction factor.

(c) The transport properties are constant with appropriate reference conditions used to evaluate these constants.

(d) The gas phase is quasi-steady relative to the drop surface changes.

(e) The processes proceed at a constant pressure which is far below

the propellant critical pressure.

Under the above assumptions, the rate of drop radius change is given by¹⁷

$$\frac{dr}{dt} = -\frac{\rho D}{2 \rho_d r} V_{sh} \ln[(1+B)(1+B_o)] , \quad (3.51)$$

where V_{sh} is the Sherwood number for mass transfer, ρD is the propellant vapor diffusivity in the ambient medium, and B and B_o are mass transfer numbers. The Sherwood number is given by

$$V_{sh} = 2.0 + 0.6 Re_d^{\frac{1}{2}} Sc_d^{\frac{1}{3}} ,$$

where $Sc_d = \frac{\mu}{\rho D}$ and $Re_d = \frac{2\rho |a+a''-\dot{V}|r}{\mu}$. The mass transfer numbers are given by

$$B = \frac{Y_{1,s} - (1-\delta_1) Y_{1,\infty}}{1 - Y_{1,s}} , \quad B_o = \frac{v_1 \hat{W}_1}{v_2 \hat{W}_2} \delta_1 Y_{2,\infty}$$

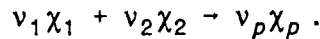
with the surface mass fraction obtained from

$$Y_{1,s} = \frac{\hat{W}_1}{\hat{W}_1 + \hat{W}_\infty \left(\frac{p}{p_v(T_d)} - 1 \right)} ,$$

where $\hat{W}_\infty$ is the local average molecular weight of all species exclusive of the drop vapor specie and $p_v(T_d)$ is the equilibrium propellant vapor pressure at temperature T_d . The parameter δ_1 is an ignition/extinction index and is taken from Law⁴⁰ with the following qualities

$$\delta_1 = \begin{cases} 1 & , \text{ignition} \\ 0 & , \text{pure vaporization} \end{cases} .$$

Ignition or extinction is determined by a correlation of numerical and theoretical results accounting for the effects of finite rate kinetics. A one-step global reaction between the drop vapor specie $[x_1]$ and the oxidizing gas $[x_2]$ is taken to be



The heat released per unit mass of drop vapor consumed at the bipropellant flame front is obtained from

$$Q_r = \frac{v_1 \Delta h_{f,1}^0 + v_2 \Delta h_{f,2}^0 - v_p \Delta h_{f,p}^0}{v_1 \dot{W}_1} .$$

This amount of heat gives a stoichiometric adiabatic flame temperature of the bipropellant system as

$$\frac{T_f - T_d}{T_\infty - T_d} = \frac{\left\{ \frac{B_o Q_r}{c_p (T_\infty - T_d)} + 1 \right\}}{\left\{ 1 + \frac{B_o}{B} (B + B_o) \right\}}$$

where T_f is the adiabatic flame temperature and T_∞ is the ambient gas temperature. Assuming uniform liquid drop temperature, an energy balance for the heat transfer processes yields

$$\frac{4}{3} \pi \rho_d r^3 c_l \frac{dT_d}{dt} - \rho_d 4 \pi r^2 \frac{dr}{dt} L(T_d) = 4 \pi r^2 Q_d \quad (3.52)$$

where c_l is the liquid specific heat (i.e., $e_d = c_l T_d$), $L(T_d)$ is the latent heat of

vaporization, and Q_d is the rate of heat conduction to the droplet surface per unit area. The heat conduction rate is given by

$$Q_d = \frac{\lambda (T_f - T_d)}{2r} V_{Nu} \ln \frac{[(1+B)(1+B_o)]}{B} ,$$

where

$$V_{Nu} = 2.0 + 0.6 Re_d^{\frac{1}{2}} Pr_d^{\frac{1}{3}} ,$$

and Pr_d and λ are effective transport parameters for the droplet gas diffusion layer. All transport coefficients are evaluated at some reference temperature and composition depending upon the specific problem.

For high ambient temperatures, experiments⁴¹ reveal the formation of an exothermic decomposition flame enveloping the hydrazine-based fuel droplets which are commonly employed in small thrusters. The existence of the decomposition flame depends on the convective environment and the decomposition kinetics. Two mechanisms should thus be considered for the fuel droplet vaporization: (1) decomposition flame within a diffusion mantle, or (2) pure diffusion flame without any decomposition. If the decomposition kinetic rate is comparable to those of the oxidation kinetics, fuel droplet life histories are obtained from a model given by Faeth⁴² for monopropellants.

3.6 Globule Acceleration and Turbulence Dispersion

A globule's acceleration is obtained by integrating Newton's second law under the assumption that the only force contribution is due to aerodynamic

drag. The resulting acceleration is

$$\frac{d\vec{v}}{dt} = \frac{3}{8} \frac{\rho}{\rho_d} \frac{|\vec{u} + \vec{u}'' - \vec{v}|}{r} (\vec{u} + \vec{u}'' - \vec{v}) C_D . \quad (3.53)$$

Acceleration of the "apparent mass" of the gas displaced by the droplet and the Basset term have been neglected. A correlation for the drag coefficient C_D is given by Rabin et al.⁴³ as

$$C_D = \begin{cases} 24 Re_d^{-0.84} & Re_d \leq 80 \\ 271 Re_d^{0.217} & 80 < Re_d \leq 10^4 \\ 2 & Re_d > 10^4 \end{cases} .$$

This correlation indirectly includes the effects of gassification in a convective flow field and the globule surface distortion. Once the globule velocity is found by integrating its acceleration with respect to time, the new globule position is determined by integrating

$$\frac{d\vec{x}}{dt} = \vec{v} . \quad (3.54)$$

A globule in a homogeneous turbulence field responds to the random field velocity. As a result, its motion undergoes random displacements that can be characterized statistically by the mean-square velocity fluctuations. The effect of turbulence fluctuation on the globule motion is obtained by employing the method of O'Rourke⁴⁴. In this method, a fluctuating velocity $\vec{u}''$ is added to the gas velocity $\vec{u}$, where each component of $\vec{u}''$ is randomly chosen from a Gaussian distribution with standard deviation $\sqrt{\frac{2}{3}k}$. This fluctuating velocity is assumed to be a piecewise constant function of time, changing discontinuously after passage of turbulence correlation time (i.e., minimum of an eddy-breakup

time and a time for the globule to traverse an eddy). As long as the computational time step is less than the turbulence correlation time, the equations of motion for a globule can be integrated in a straightforward manner. When this is not the case, random velocity and position changes are sampled from assumed probability distributions. These changes are then added to the deterministic globule velocity and position. Also, this same velocity fluctuation is employed when calculating the liquid/gas turbulence KE source term and a globule's Reynolds number.

This completes the model formulation. The sub-models described, are continually being updated. Any updates can be consistently incorporated within the framework provided herein. The liquid globule sub-models describe the physics taken place at the liquid/gas interface. Hence, output results from these sub-models allow the liquid/gas interface exchange rates to be computed. The next section describes the solution procedure employed.

4 SOLUTION PROCEDURE

4.1 Selection of a Computational Scheme

The choice of a computational technique to solve the mathematical model formulated herein is dictated by the need for an efficient yet flexible computer code. Currently, three methods are available for the solution of the liquid globule conservation equation. They consist of moment equation methods⁴⁵ (ME), the globule state discretization (GSD) method⁴⁶, and liquid parcel (LP) methods⁴⁷. A choice among the three is arrived at in what follows.

The ME methods solve mass, momentum, and energy equations obtained from the liquid globule conservation equation by taking appropriate moments. This is analogous to a continuum field description of the liquid globule assembly. Finite difference techniques are used to solve the moment equations. The liquid/gas interfacial sources are evaluated by assuming a form for the globule distribution function.

In the GSD method, the portion of the globule state space occupied by the globule is sub-divided into computational cells. Finite difference techniques are used to discretize the globule conservation equation in these cells. The value of the globule distribution function is tracked in time from cell to cell.

In parcel methods, the continuous globule distribution is approximated using a finite number of computational parcels. Each parcel represents a number of globules of identical states. The parcel trajectories in the globule state space are globule characteristic paths. It can be shown¹⁹ that this representation is equivalent to replacing the continuous globule distribution function with Dirac delta functions. Hence, the parcels behave as localized point sources traveling in a gaseous environment.

The disadvantage of the ME methods is that to evaluate the exchange rates, a globule distribution function must be assumed. Also, in order to simulate a polydispersed spray, several monodispersed sprays must be superposed. This requires the solution of moment equations for each distinct class of droplets as determined by the initial size distribution. An advantage of the ME methods is that the same computational scheme can be used for both the gas and liquid phases. As for the GSD method, the primary disadvantage is the large amount of computer storage required due to the many state variables employed. This disadvantage is offsetted somewhat by the direct evaluation of the globule distribution function. The parcel methods do not suffer from numerical smearing or excessive grid distortions since parcels are assumed to follow globule characteristic paths. However, a complete reconstruction of the globule distribution function requires an ensemble averaging of a large parcel population over many computations. For the present application, details of the globule

distribution are not required. What is required, is an accurate description of the evolution of the globule state variables along globule characteristic paths. Thus, a parcel method is the method of choice.

Dukowicz¹⁹ has extended the parcel method by applying the ideas of the Monte Carlo method to create what is called the stochastic parcel method. In this method, droplet state variables at the time of formation are assigned by using a Monte Carlo sampling technique for given probability distributions. The droplet number distribution function is obtained by averaging over a long time in steady-state calculations, or over many calculations in unsteady problems.

Many techniques are available for solving the gas phase governing equations. A robust and modularized technique is desirable. The computational procedure chosen is based on the KIVA-II code with some extensions. KIVA-II solves the unsteady equations of motion of a turbulent, chemically reactive mixture of ideal gases, coupled to the discrete parcel technique for a single-component vaporizing fuel spray. The gas phase solution procedure is based on a finite volume method called the ALE (arbitrary Lagrangian-Eulerian) method⁴⁸. Spatial differences are formed on a finite difference mesh that subdivides the computational region into a number of small cells. The positions of the cell vertices may be arbitrarily specified functions of time, thereby allowing a Lagrangian, Eulerian, or mixed description. Adaptation of the KIVA-II computation-

al framework to the present formulation is now described.

4.2 The Discrete Parcel Method

In the discrete parcel method, the continuous globule distribution function is approximated by a discrete distribution:

$$F(\vec{S}, t) = \sum_{p=1}^{NP} N_p \delta(\vec{S} - \vec{S}_p) . \quad (4.1)$$

Each parcel p is composed of a number of globules N_p having identical state variables $\vec{S}_p$. Analogous expressions may be written for the $g(\vec{S}, t)$ and $f(\vec{S}, t)$ distributions. This effectively sub-divides the liquid mass into groups of locally monodispersed discrete globule clouds. A parcel follows the globule characteristic paths in the globule state space and interacts with the gas phase in a localized point source fashion. Hence, when equation (4.1) is employed in the expressions for the liquid/gas interface exchange rates (sect. 2), the integrals are quickly evaluated by a straightforward accounting procedure. The number of globules represented by each computational parcel is initially assigned at the point of injection and is allowed to change depending upon the various processes undergone by a parcel.

4.2.1 Parcel Injection

Computational parcels are introduced within the computational domain at the point of injection. These parcels must be injected in such a way that a uniform distribution of globule properties is obtained. The method that is used assures that a continuous train of discrete parcels will emerge from the point of injection.

At the point of injection, each parcel must be assigned a certain amount of mass along with the initial globule state variables. The initial size of a globule is usually specified as the circular orifice radius or its equivalent for non-circular slots. Initial globule velocities are estimated from mass conservation considerations. The globule mass flux at the injector exit plane may be written as

$$\frac{d}{dt} \sum_{p=1}^{NP} \int m N_p \delta(\vec{S} - \vec{S}_p) d\vec{S} = \dot{M}_I ,$$

where $\dot{M}_I$ is the liquid mass flow rate across the injector face and m is the mass of a globule. Letting the injected parcel mass M_p be constant results in

$$M_p \text{PRATE} = \dot{M}_I ,$$

where

$$M_p = m N_p = \frac{4}{3} \pi \rho_d r^3 N_p ,$$

and PRATE is the parcel injection rate (i.e., $\frac{d(NP(t))}{dt}$). The parcel injection rate

is chosen in such a way that a continuous train of parcels is issued from the injector. An expression that satisfies this requirement is

$$PRATE \leq \frac{v_{inj}}{2r} ,$$

where v_{inj} is the injection velocity. The number of globules per parcel is thus obtained.

4.2.2 Liquid Stream Impingement Calculation

The parcel representation of the globule number distribution function allows a very simple solution procedure for the effects of impingement collision (i.e., an evaluation of the collision source term). A computational sequence proceeds as follows for each pair of unlike parcels belonging to the intact liquid core.

(1) The criteria for impending collision (eq. 3.22) is checked and if satisfied, the collision computations proceed for this globule pair.

(2) Mass average interface quantities are now obtained.

(3) The mixing ratio (f_{mix}) is calculated according to

$$f_{mix} = \max(N_1, N_2) \frac{\bar{v}_{21} \cdot \bar{e}_{12} \Delta t \pi (r_1 + r_2)^2}{V_{12}}$$

where the subscripts 1 and 2 refer to the parcel pair and V_{12} is the liquid volume occupy by the parcel pair. This mixing ratio is constrained to be less than one.

(4) The number of globules from each parcel that interact through collision is calculated from

$$n_{coll} = \min(N_1, N_2) f_{mix} .$$

This number of globules is subtracted from each parcel and two new parcels are created with attributes reflecting the outcome of the collision (eq. 3.29).

(5) Finally, all like parcels which are at the same location are arithmetically averaged into a single parcel (i.e., coalescence).

There is a time step limitation on the above procedure. That is, the time step Δt must be chosen so that $f_{mix} \leq 1$. Computational procedures for the other liquid parcel sub-models are straightforward (see Ref. 29 for examples) except for atomization and will not be repeated here. Suffice to say that the equations for drop combustion (eqs. 3.51 and 3.52) are integrated implicitly via a predictor-corrector scheme. Equation (3.53) for the globule acceleration is integrated implicitly due to its strong coupling with the gas velocity and the globule position (eq. 3.54) is updated in an explicit fashion. A second-order interpolation technique is used to map the globule characteristic paths onto the gas phase computational mesh when locating appropriate gas upstream properties to use for evaluating the liquid/gas exchange rates. The method that is employed for the atomization/breakup calculation is outlined next.

4.2.3 Atomization/Breakup Calculation

Globule breakup occurs if and only if the distortion parameter y exceeds unity. To update the values of y and its time rate of change, the exact solution of equation (3.40) is employed under the assumption of constant coefficients during the current computational cycle. The procedure is as follows.

(1) For each parcel, the values of y and $\dot{y}$ are first updated due to impingement collision. These updated values now become initial conditions (eq. 3.39) for the exact solution of equation (3.40).

(2) The amplitude of the exact solution to y is checked to see whether or not breakup is possible during this current computational cycle. If breakup occurs, the Sauter mean radius (SMR) of the product drops is calculated (eq. 3.44). If breakup does not occur, the distortion and oscillation parameters are updated according to the exact solution. If breakup occurs, steps (3-4) are followed.

(3) The velocity (eq. 3.42) normal to the path of a product drop is now obtained. This velocity increment is randomly distributed about the normal directions to the relative velocity vector of the parent globule. The velocity of the product drops are now obtained by adding this velocity increment to the parent globule velocity vector.

(4) The radius of the product drops is then chosen randomly from a given distribution with the calculated SMR. To conserve mass, the number of globules

associated with the computational parcel is adjusted. The distortion and oscillation parameters of the product parcel are set to zero. Also, this product parcel is tagged as belonging to the dispersed liquid cluster.

The number of parcels produced from the breakup of globules belonging to one intact liquid core parcel is a free parameter. This number is chosen in such a way that a reasonable resolution of liquid properties is obtained. Its value is input for each specific problem and the number of globules per product parcel is adjusted so that mass is conserved.

4.3 The ALE Method

The original ALE method is described in detail by Hirt et al.⁴⁸ and will be delineated only briefly here. Arbitrary Lagrangian-Eulerian zoning permits optimal use of computational zones, allows for the calculation of flows involving curved or moving boundaries, and makes possible calculations with minimum computational diffusion without excessive grid distortions. KIVA-II uses the ALE computational mesh together with a SIMPLE⁴⁹-styled iterative pressure correction treatment. The temporal differencing is performed with respect to a sequence of discrete times or cycles. A cycle proceeds in three stages. Stages A and B together constitute a Lagrangian calculation in which computational cells move with the fluid. Stage A is a calculation of source terms due to the liquid/gas

interfacial exchanges and gas phase chemical reactions. Stage B calculates in a coupled, implicit fashion the acoustic mode terms (i.e., the pressure gradient in the momentum equation and velocity dilatation terms in mass and energy equations), the liquid/gas momentum source term, and the terms due to diffusion of mass, momentum, and energy. Stage B also calculates the remaining source terms in the turbulence equations. In stage C, the flow field is frozen and rezoned or remapped onto a new computational mesh.

A three-dimensional Cartesian computational mesh made up of hexahedrons is employed. Axisymmetric cylindrical geometries are handled through the use of periodic boundary conditions. A staggered mesh arrangement is employed whereby velocities are located at the cell vertices and thermodynamic quantities are located at cell centers. Spatial difference approximations are constructed by the control volume or integral balance approach, which largely preserves the local conservation properties of the differential equations. The discretized form of the actual equations will not be given here but can be found in Ref. 29. A one-dimensional model is used to illustrate the features of the ALE method.

Consider the one-dimensional motion of a non-vaporizing spray in an isothermal gas. The gas velocity magnitude and gradients are assumed to be small so that viscous effects are negligible. A suitable set of equations (sect. 3.1)

for this problem is:

mass conservation

$$\frac{d}{dt} \int_V \rho dV + \oint \rho u(u-U) dA = 0$$

momentum balance

$$\frac{d}{dt} \int_V \rho u dV + \oint \rho u(u-U) dA = - \oint p dA + \int_V F^s dV$$

energy conservation

$$T = \text{constant} .$$

U is the surface velocity of the control volume and F^s is the spray/gas momentum exchange. The volume is discretized with a staggered arrangement as shown in Figure 5. A computational mesh with uniform cross-sectional area A is used. The time interval $\Delta t = t^{n+1} - t^n$ is the timestep, and the integer n is the

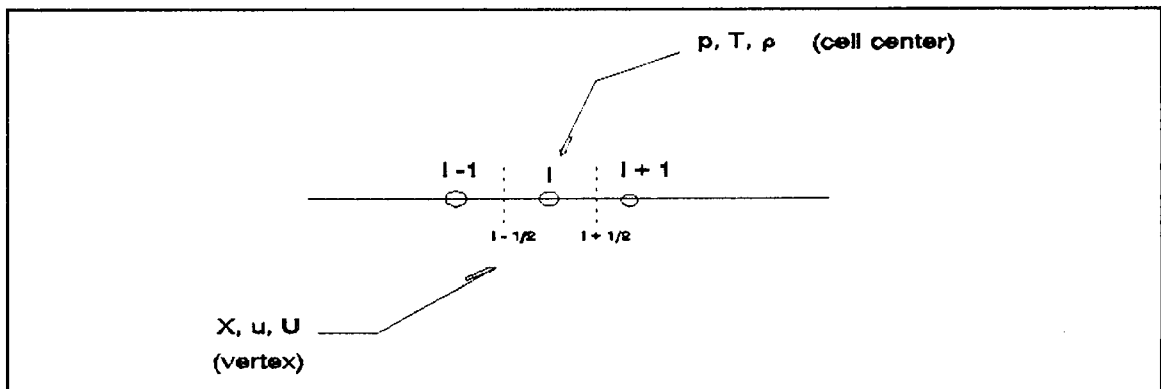


Figure 5. Staggered mesh arrangement for ALE scheme (1-D).

cycle number. Cell centers are indexed by the integer i with vertices labeled as $i + \frac{1}{2}$. The mass conservation equation is integrated over these cells with the

momentum equation integrated over a momentum cell centered about a vertex.

The discretized equations follow.

1. Lagrangian mesh difference equations

The Lagrangian mesh employs vertices moving with the local gas velocity (i.e., $u=U$). Stage A difference equations are:

mass

$$M_i^A = M_i^n = \int_{V_i^n} \rho_i^n dV .$$

Thus the mass in a cell is constant as it should be in the absence of mass sources. The stage A volume is the same as that of the previous cycle.

momentum

$$(M'u)_{i+\frac{1}{2}}^A - (M'u)_{i+\frac{1}{2}}^n = \int_n^A \int_{V_i'} F_{i+\frac{1}{2}}^S dV dt$$

where $M'_i = \frac{1}{2}(M_i + M_{i+1})$ is the mass associated with a vertex. The spray momentum source term is usually strongly coupled to the gas momentum thereby necessitating an implicit treatment. This source term is linearized in the form

$$F_{i+\frac{1}{2}}^S = F_{0,i+\frac{1}{2}}^S + \left(\frac{\partial F^S}{\partial (\rho u)} \right)_{i+\frac{1}{2}} (\rho u)_{i+\frac{1}{2}}^A$$

where F_0^S is the constant part of F^S . Thus, the resulting stage A discretized momentum equation is

$$\frac{[1 - (\frac{\partial F^S}{\partial(\rho u)})_{i+\frac{1}{2}} \Delta t](M'u)_{i+\frac{1}{2}}^A - (M'u)_{i+\frac{1}{2}}^n}{\Delta t} = F_{0,i+\frac{1}{2}}^S (V_i')^n$$

where the slope $\frac{\partial F^S}{\partial(\rho u)}$ is constructed in such a way that its value is negative.

This is required for stability reasons (see Patankar⁴⁹).

Stage B includes the pressure gradient and velocity dilatation effects. The discretized equations are:

mass

$$M_i^B = M_i^A = \rho_i^B V_i^B$$

momentum

$$\frac{[1 - (\frac{\partial F^S}{\partial(\rho u)})_{i+\frac{1}{2}} \Delta t](M'u)_{i+\frac{1}{2}}^B - (M'u)_{i+\frac{1}{2}}^A}{\Delta t} = [\phi_p(P_{i+1}^B - p_i^B) + (1 - \phi_p)(p_{i+1}^n - p_i^n)]A$$

where ϕ_p is an implicit weighting factor between 0 and 1. In particular, $\phi_p=0$ leads to an explicit scheme, and $\phi_p=1$ to a fully implicit scheme. An explicit scheme has to satisfy certain stability restrictions whereas a fully implicit scheme is constrained by accuracy and computational efficiency requirements. A variable implicitness depending upon local conditions may be employed to capitalize on the favorable qualities of both fully implicit and explicit schemes.

The Stage B pressure is obtained iteratively (i.e., SIMPLE procedure) by

including the following auxiliary equations:

equation of state

$$P_i^B = \frac{M_i^B}{V_i^B} R_g T$$

conservation of volume (velocity dilatation)

$$V_i^B = V_i^n + A \Delta t [u_{i+\frac{1}{2}}^B - u_{i-\frac{1}{2}}^B] .$$

These equations along with the momentum equation can be manipulated to obtain a direct equation for the pressure. Once the phase B volume is available, the phase B mass density directly follows. The Lagrangian mesh vertex positions are obtained from

$$x_{i+\frac{1}{2}}^B = x_{i+\frac{1}{2}}^n + u_{i+\frac{1}{2}}^B \Delta t .$$

2. Mesh rezoning

Usually a Lagrangian mesh results in large grid distortions thereby requiring some sort of rezoning (either Eulerian or arbitrary). In the ALE scheme, the rezoning is performed as follows. The required vertex velocity (U) is used to set the vertex position as

$$x_{i+\frac{1}{2}}^{n+1} = x_{i+\frac{1}{2}}^n + U_{i+\frac{1}{2}} \Delta t$$

In going to this new desired position from the Lagrangian position, a certain amount of cell volume is swept out by a cell face carrying with it mass and

momentum. Hence, a convective fluxing procedure must be engaged. The procedure employed in the KIVA-II code is called a quasi-second order upwind (QSOU) scheme. This QSOU has first order spatial truncation errors and is monotone. A monotone scheme has the property that it introduces no new maxima or minima in the computed solution. This quality is desirable when tracking fronts such as shocks and flame regions. Details of its application may be obtained by consulting Ref. 29. Suffice to say that this procedure is handled in an explicit subcycled manner so that the Courant time step restriction (CFL criteria) does not impair the computational time step.

This 1-D model problem just explained shows the essential steps in the ALE method. Application of this technique to the complete set of equations is performed in a very similar fashion.

4.4 Initial and Boundary Conditions

KIVA-II employs a time-accurate computational scheme for solving equations describing transient processes. Therefore, an initial flow field is needed to start the time marching sequence. For most applications, a steady-state solution is required. This steady-state is arrived at by starting from an initial guess of the flow field. The guessed flow field is usually a stagnant medium at some appropriate pressure, temperature, and turbulence intensity.

There are two types of boundary conditions that are needed in order to perform a calculation. First, physical boundary conditions must be provided to describe the physical bounding walls. Second, numerical boundary conditions are needed in order to describe computational boundaries such as inflow or outflow.

In the present applications, turbulent law-of-the-wall velocity conditions with adiabatic walls are specified. On turbulent law-of-the-wall boundaries, the normal gas velocity is set equal to the normal wall velocity and the tangential components are determined by matching to a logarithmic profile⁵⁰. The boundary conditions for the individual species are zero gradients of the mass fractions at the walls, corresponding to chemically-neutral surfaces and no fluxes through the walls. In calculations of turbulent flow, boundary conditions are also needed for the turbulence kinetic energy and its dissipation rate. These are taken to be zero normal gradient of turbulence kinetic energy and equilibrium between generation and dissipation of turbulence.

In bipropellant spray combustion calculations, there are usually no gas inflow boundaries. The outflow boundary is assumed to be subsonic. At the outflow boundary, the pressure is specified along with zero gradients for the velocity. This kind of outflow treatment is susceptible to acoustic wave reflections which can affect convergence rate to a steady-state. Artificial devices are

sometimes necessary in order to alleviate this problem. Usually, a lengthening of the actual outflow boundary reduces acoustic wave reflection.

Boundary conditions are also needed for the globule conservation equation. The conditions at the point of injection have already been indicated. A globule/wall interaction model is needed in order to describe the outcome of a collision between a globule and a wall. The model employed is an extension of that described by Naber and Reitz⁵¹. In this model, it is assumed that an incident globule leaves tangent to the wall in the manner of a liquid jet. It is also assumed that the angle, ψ , at which an impinging globule flows along the wall can be found from theoretical analysis of the impingement of a liquid jet on an inclined wall. The geometry of this liquid jet analogy model is sketched in Figure 6. An expression for the wall flow angle is obtained from

$$\psi = -\frac{\pi}{\beta} \ln[1 - RND(1 - e^{-\beta})] ,$$

where RND is a random number uniform on the interval (0,1) and β is obtained from

$$\sin \alpha = \left[\frac{e^{\beta} + 1}{e^{\beta} - 1} \right] \frac{1}{1 + \left(\frac{\pi}{\beta} \right)^2} ,$$

where α is the wall inclination angle relative to the incoming globule direction. Wachters and Westerling⁵² described in detail the phenomena observed when water drops impinge on heated walls. The drop Weber number, $We_n = \rho_d v_n^2 \frac{r}{\sigma}$,

is an important parameter of the problem (v_n is the drop velocity component normal to the surface). There is a critical Weber number separating the regime of wall jet flow and globule rebounding. At an approach Weber number less than critical, globules rebound from the wall and beyond the critical Weber number, the liquid spreads out in a layer on the wall. The Naber and Reitz model is extended to include this critical Weber number dependence. Estimates of the critical Weber number (usually on the order of 50) can be obtained from Hebrard and Lavergne⁵³. It should be noted that this globule/wall model does not account for heat transfer effects.

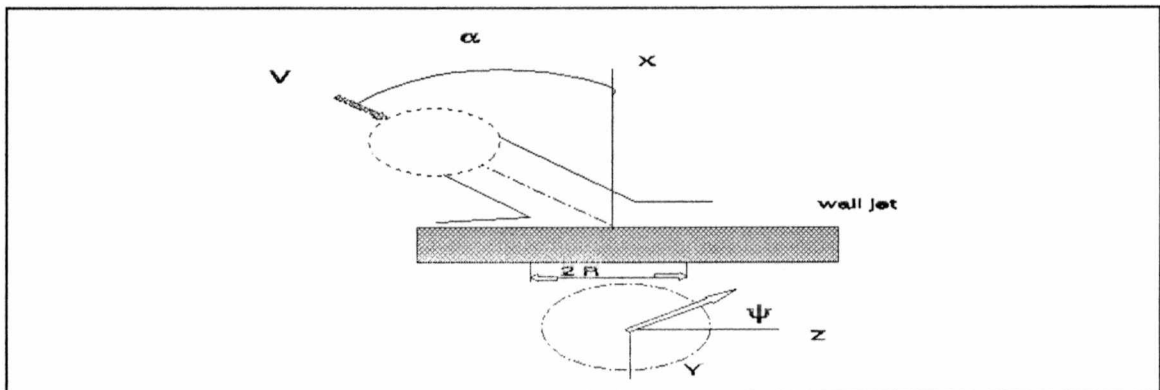


Figure 6. Schematic of spray/wall jet interaction model.

4.5 Summary of the Solution Procedure

The overall solution process is schematically depicted in Fig. 7. A top-to-bottom flow encompassing the primary steps in the solution is shown. The gas dynamic flow solver (ALE) is coupled to the discrete parcel technique for the

liquid phase and a gas chemistry package. This coupling can be performed in many ways depending upon the specific application. The next section illustrates some bipropellant spray combustion related applications.

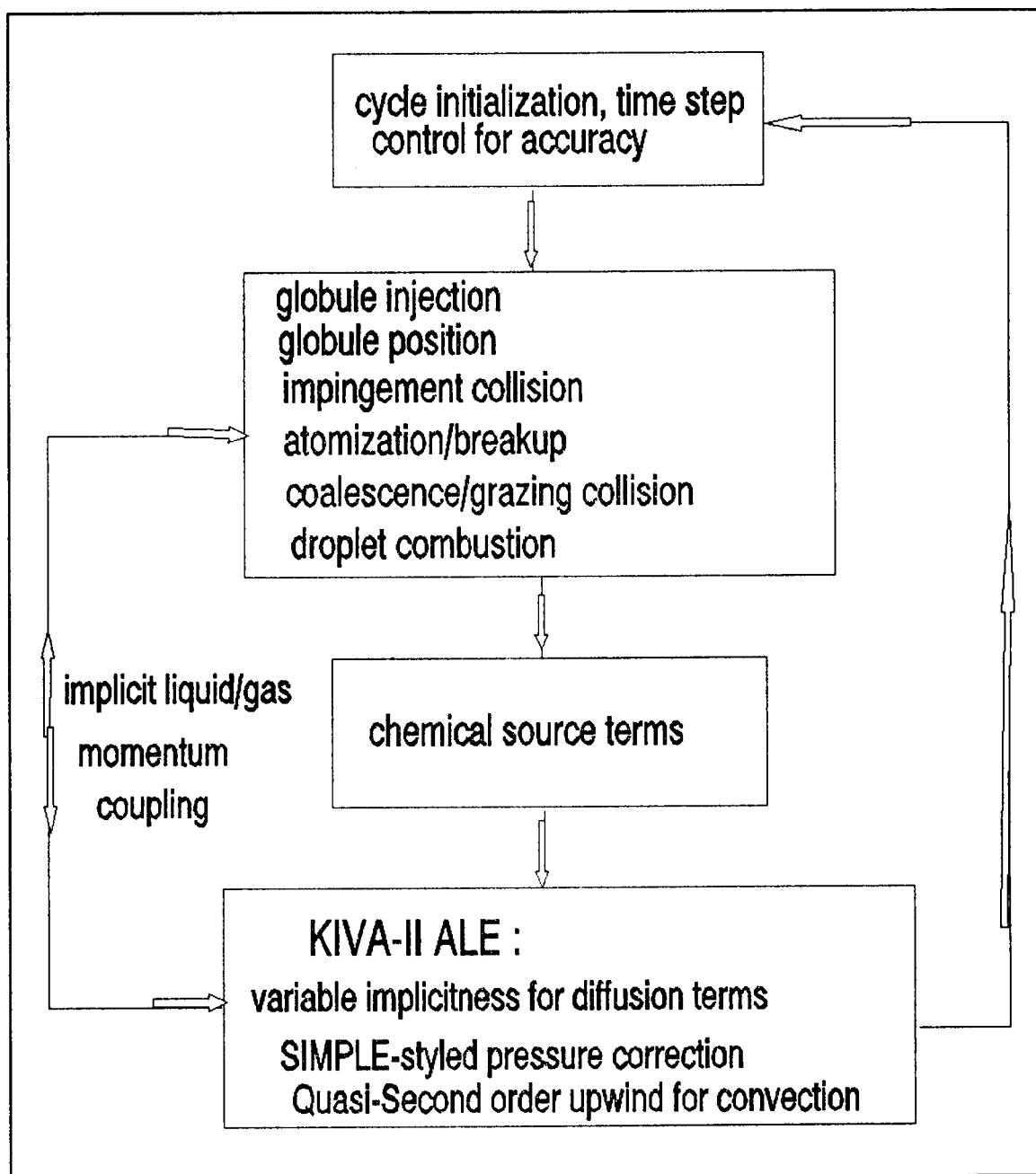


Figure 7. Overall flow diagram for adapting the KIVA-II code to the present formulation.

5 APPLICATIONS

5.1 Impinging Doublet Spray Structure

The present technique is applied to the study of the spray structure produced by impinging stream injectors. Two configurations are considered. The first consists of the impingement of two like-liquid streams (like-doublet) in an initially quiescent, unconfined, standard-atmospheric gas. A second configuration involves the impingement of two unlike-liquid (unlike-doublet) streams in an initially quiescent, confined standard-atmospheric gas. Under these conditions, vaporization of the spray drops is not significant. Hence, spray combustion and gas phase chemistry effects were ignored for these two cases. The emphasis is on the gross spray structure (i.e., intact liquid core length, cone angle, and drop size distribution) and the momentum exchange with the gas. For the confined case, the interaction of a spray with a wall is appraised.

Like-doublet stream impingement

Heidmann et al.⁹ reported on the spray formed by two impinging water jets at different impingement angles and injection velocities. Single-exposure microflash photographs were taken of the sprays. This allows the spray patterns to be qualitatively studied. The spray cone angle can be estimated from the photographs, but no data is provided about average drop size and distribution.

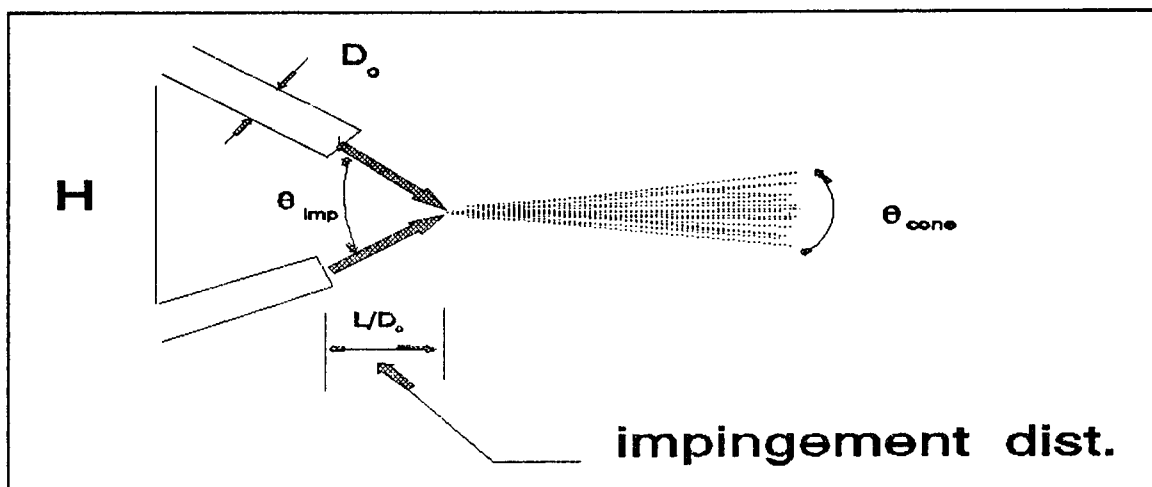


Figure 8. Like-doublet impinging stream injector.

Figure 8 depicts the like-doublet injector employed in this study. The impingement distance (i.e., free-stream jet length) was kept constant for different impingement angles by varying the distance H between the two circular orifice tubes. A turbulent jet is said to be produced by this configuration for jet velocities of interest ($v_{inj} > 600 \text{ cm/s}$). Some of the photographs taken by Heidmann are reproduced in Figures 9 and 10. Figure 9 illustrates the effect of impingement angle on spray pattern for angles of 30, 60 , and 90 degrees. These photographs show a shorter distance for complete atomization as impingement angle is increased. The variation in the spray pattern resulting from changes in jet velocity at a 60 degree impingement angle is shown in Figure 10. It can be seen that the spray pattern is not substantially altered by jet velocity.

A simulation of two like stream impingement was performed with liquid hydrazine (N_2H_4) substituted for water. Even though the current model is

formulated for two immiscible liquids, the computed results should be of some use. The computed spray structures are to be compared with the photographs taken by Heidmann. Axisymmetry was assumed and the computations were

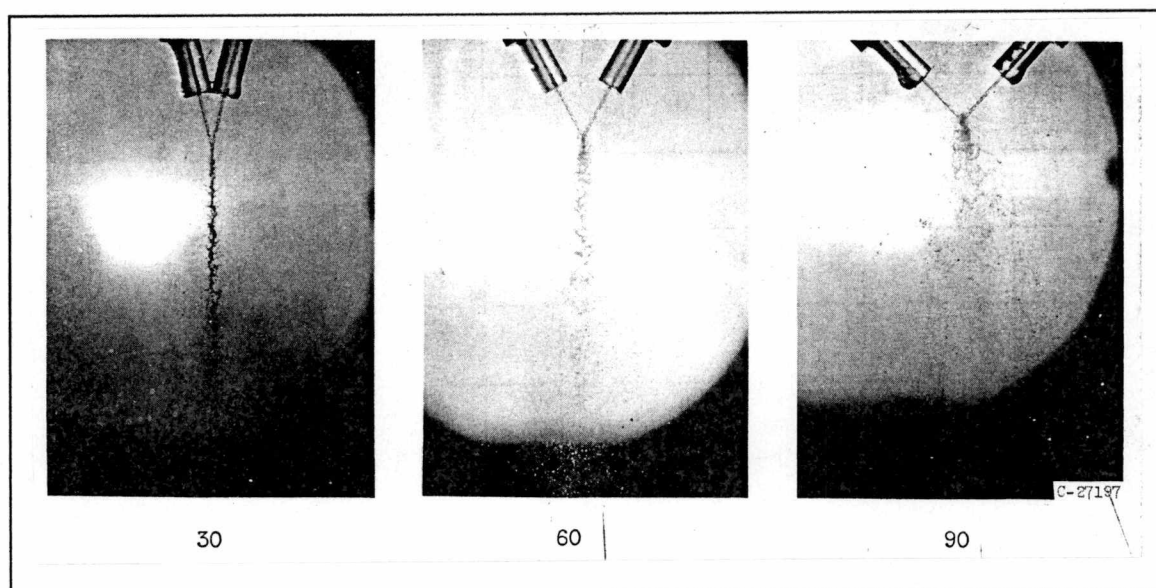


Figure 9. Effect of impingement angle on spray pattern. Jet diameter, .064 cm; jet velocity, 1827 cm/s; fluid, water.

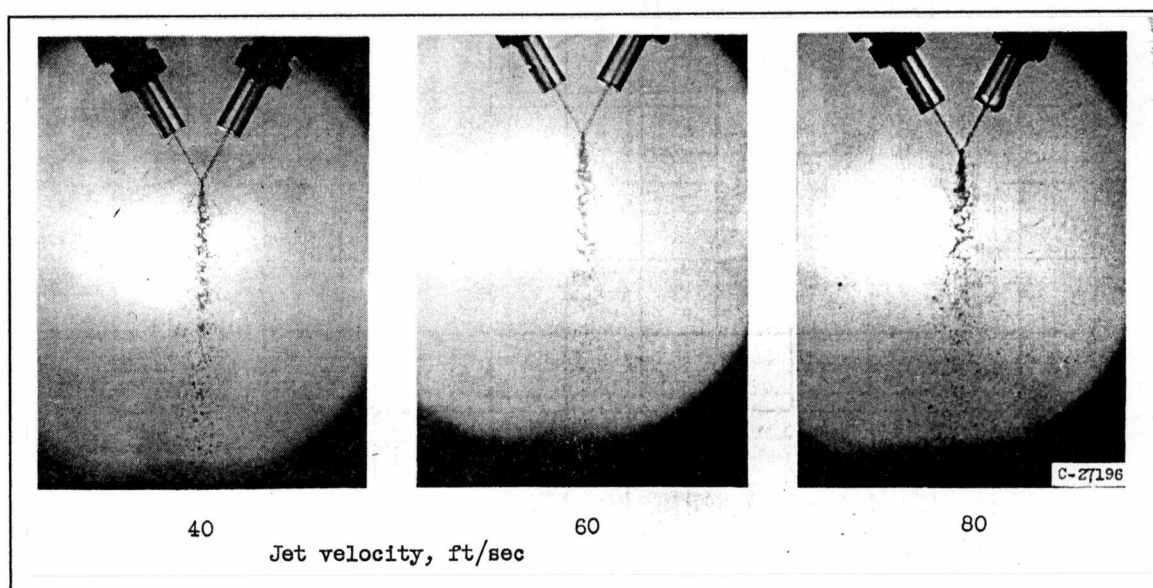


Figure 10. Effect of jet velocity on spray pattern for 60 degree impingement.

carried out in a cylindrical domain with a radius of 4 cm and a length of 15 cm. The mesh spacing is uniform with 20 radial and 60 axial computational cells. Figure 11 illustrates the computational domain along with the locations of the outflow boundaries. Initially, the computational domain consisted of quiescent gas (N_2) at a pressure of 1 atm and a temperature of 300 K.

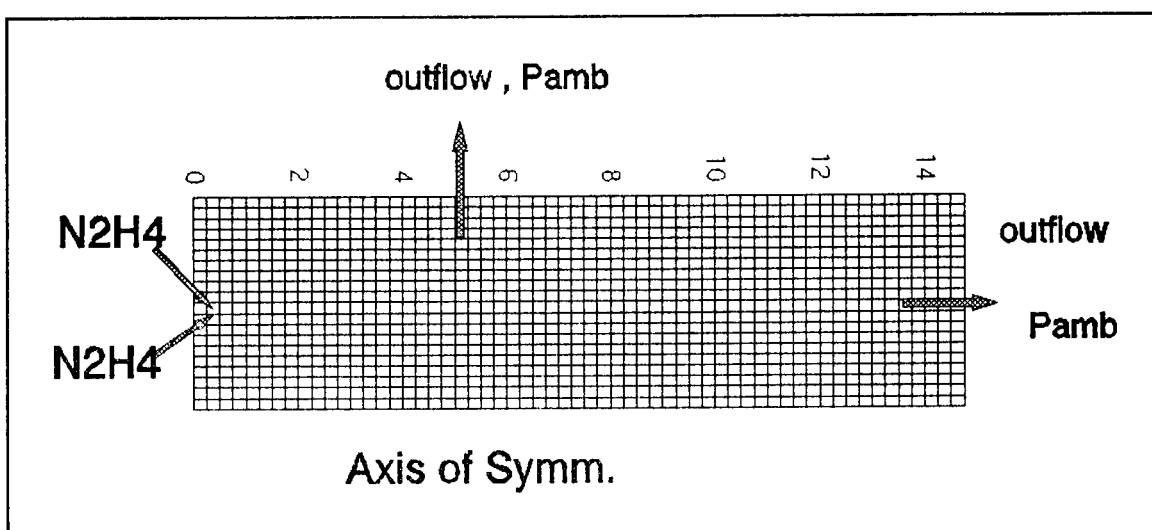


Figure 11. Axisymmetric computational domain for N_2H_4 like-doublet impingement.

Table I presents the conditions for this simulation. The N_2H_4 liquid properties are almost identical to those of water at 300 K thereby allowing a direct comparison of the spray structures. Also included in Table I is the Sauter mean radius (SMR^*) obtained from the correlation of Dickerson¹¹ for like-doublet injectors using water. An SMR is the radius of a drop whose ratio of volume to surface area is the same as that of the entire spray. The cumulative size distribution function employed is of the form

$$G(r) = 1 - \cos^{4.5} \left(.221 \pi \frac{r}{r_{32}} \right)$$

where r_{32} is the Sauter mean radius defined by

$$r_{32} = \frac{\int_0^\infty r^3 \frac{dG(r)}{dr} dr}{\int_0^\infty r^2 \frac{dG(r)}{dr} dr}.$$

This size distribution approximates the popular Rosin-Rammler distribution. The correlation of Dickerson is actually given in terms of a volume-mean radius but using the above size distribution, an equivalent SMR was obtained.

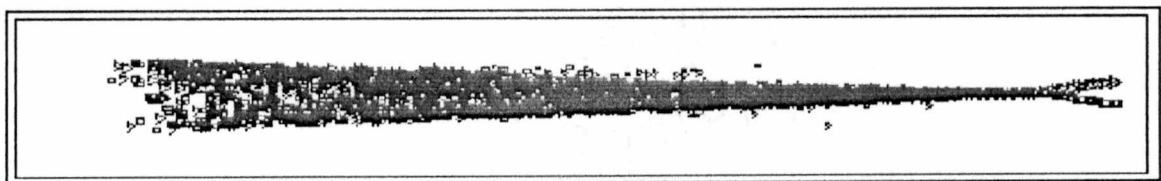
Table I. Conditions for N₂H₄ like-doublet stream impingement.

$\mu_{\text{liquid}} = .97 \text{ centipoises}; \sigma_{\text{liquid}} = 75 \text{ dynes/cm}; \rho_{\text{liquid}} = 1 \text{ g/cc}; D_o = .064 \text{ cm}; L/D_o = 10$				
θ_{imp}	v_{inj} (cm/s)	Mass Flow (g/s)	SMR* (cm)	θ_{cone} (Ref. 9)
30	1827	12	.0043	5
90	1827	12	.0027	20
60	1827	12	.0035	10
60	1218	8	.0050	10
60	2436	16	.0028	10

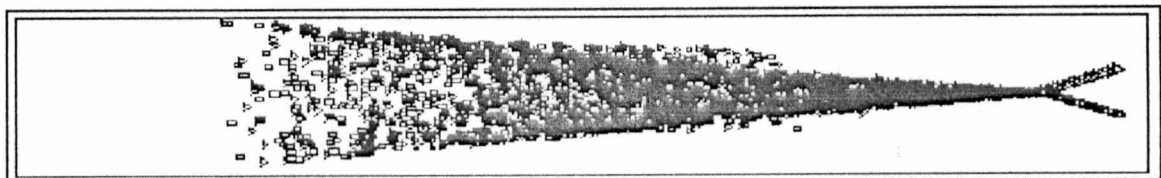
Table I contains the spray cone angles determined from the photographs of Heidmann. The cone angle given is defined as the angle formed by two straight lines drawn from the point of impingement to cut the spray boundary 4

cm downstream of impingement.

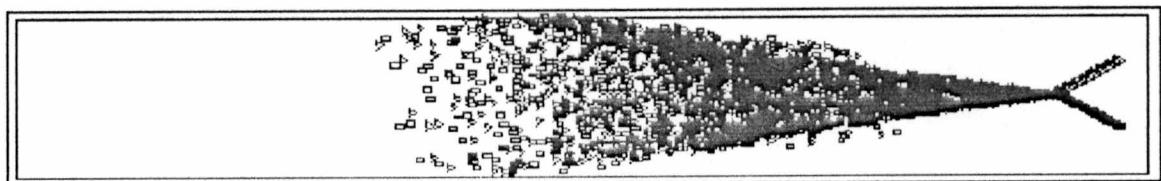
Figure 12 shows a series of parcel plots comparing the spray structure at various impingement angles. The computed spray structures are in qualitative agreement with the photographs of Heidmann. Furthermore the computed spray cone angles agree very closely with those estimated from the photographs.



(a) 30 dgr. impingement; computed cone angle, 6 dgr.



(b) 60 dgr. impingement; computed cone angle, 11 dgr.

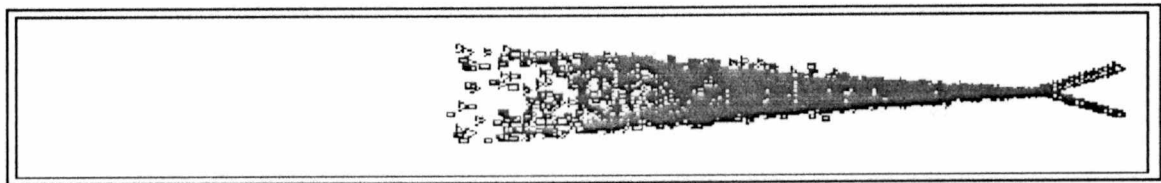


(c) 90 dgr. impingement; computed cone angle, 21 dgr.

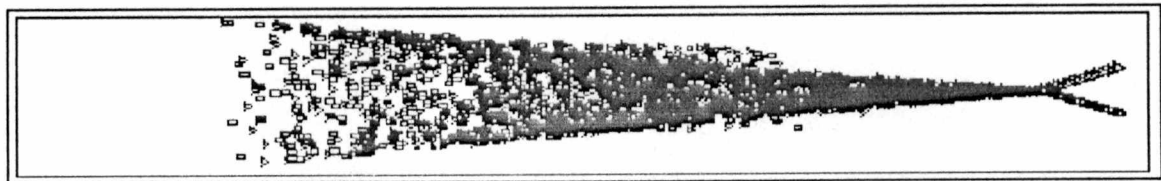
Figure 12. Parcel plots illustrating the effect of impingement angle on spray structure. The symbol sizes are proportional to liquid globule size.

The effect of varying the injection velocity on the spray structure is depicted in Figure 13. Again, good qualitative agreement is obtained with the photographs of Heidmann. For a given impingement angle, varying the injection

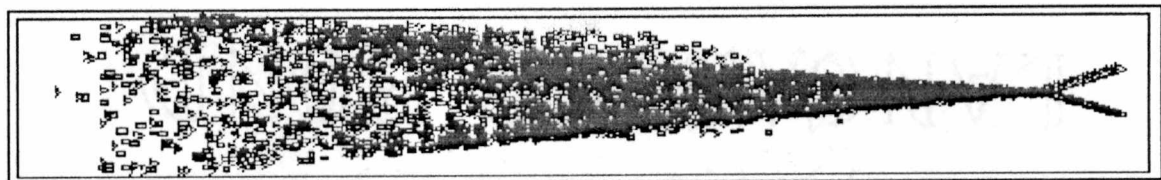
velocity has no significant effect on the spray structure. This result is only valid for the range of injection velocities considered. A fully developed spray is obtained with this range of injection velocities. For lower velocities, the disintegration of a liquid sheet by impact waves may not be possible (i.e., the impact Weber number is below the critical value).



(a) 60 dgr. impingement; injection velocity, 1218 cm/s; cone angle, 12 dgr.



(b) 60 dgr. impingement; injection velocity, 1827 cm/s; cone angle, 11 dgr.



(c) 60 dgr. impingement; injection velocity, 2436 cm/s; cone angle, 13 dgr.

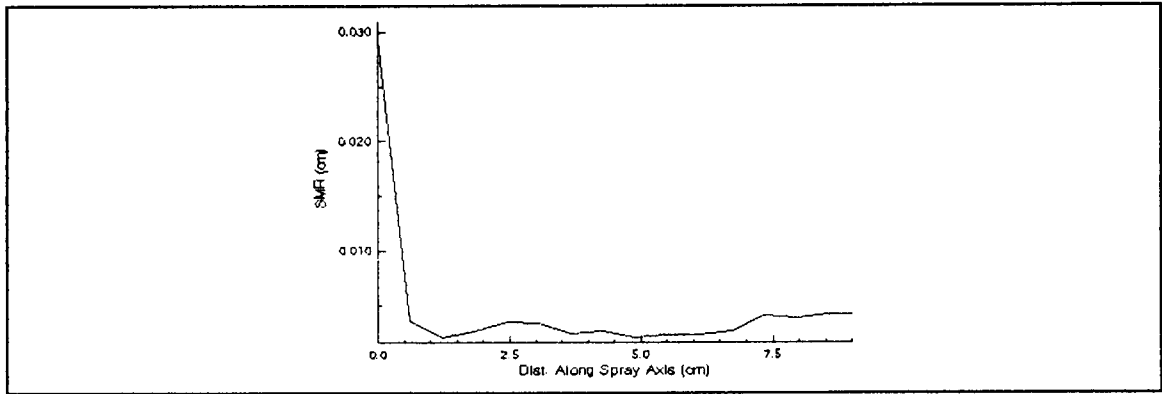
Figure 13. Parcel plots illustrating the effect of varying injection velocity on spray structure for 60 degree impingement.

The computed variations of drop size (SMR) along the spray axis from the point of impingement are depicted in Figures 14 and 15. Since globules having an initial radius equal to the orifice radius were injected, the SMR plots originate with the orifice radius. The computed globule size is that obtained after 10 ms

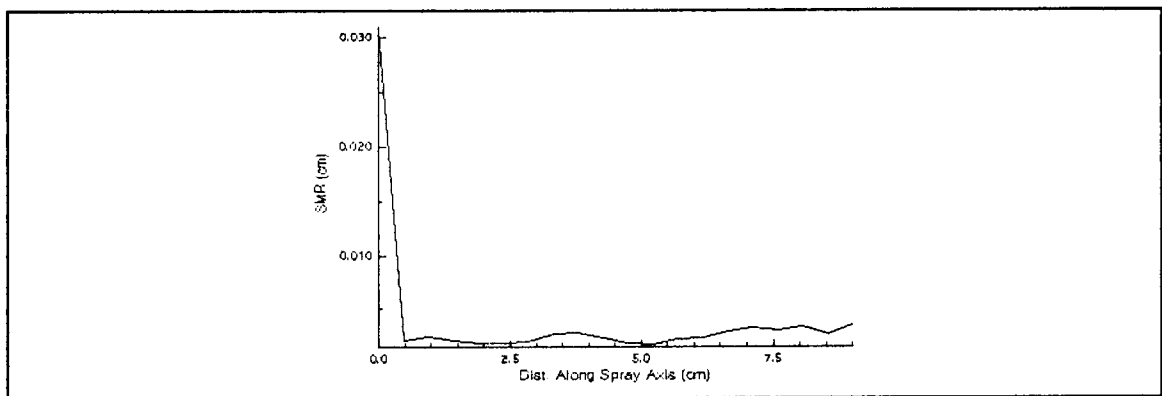
without time averaging over the spray crosssection at each axial position. Hence, the fluctuations are attributed to numerical under-sampling. Due to globule breakup, the SMR decreases rapidly within a short distance from the impingement point and then gradually increases.

The downstream SMR distribution is fairly uniform for the 60 and 90 degree impingements. For the 30 degree case, there seems to be a significant amount of coalescence and secondary drop breakup following the primary globule breakup. This is probably due to the higher concentration of globules produced in the 30 degree case. The level of computed drop sizes seems to agree fairly well with the correlation of Dickerson. As expected, the drop size is inversely proportional to the injection velocity. Increasing the impingement angle results in a decrease of the drop size. This trend does not seem to be linear.

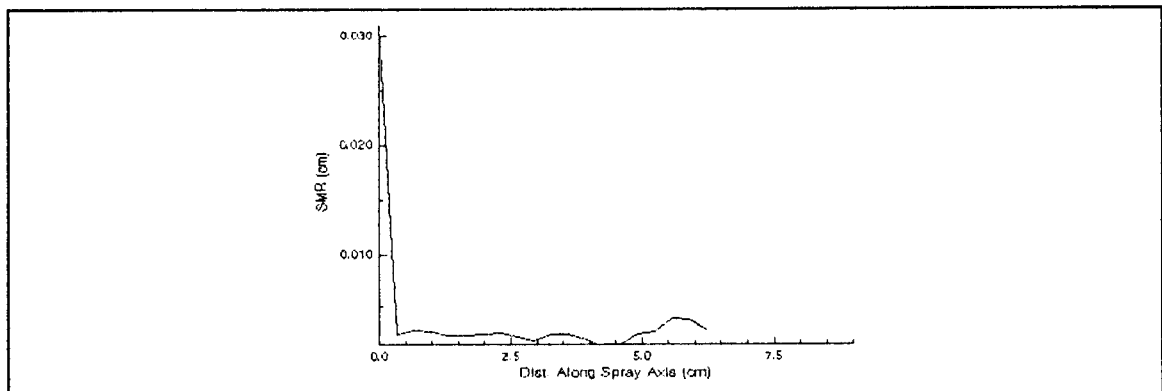
There is a region near the impingement point where a rapid change in globule size occurs. The length of this region (breakup length) is inversely proportional to the impingement angle. Varying the injection velocity does not seem to produce significant changes in this breakup length.



(a) 30 dgr. impingement; $v_{inj} = 1827$ cm/s

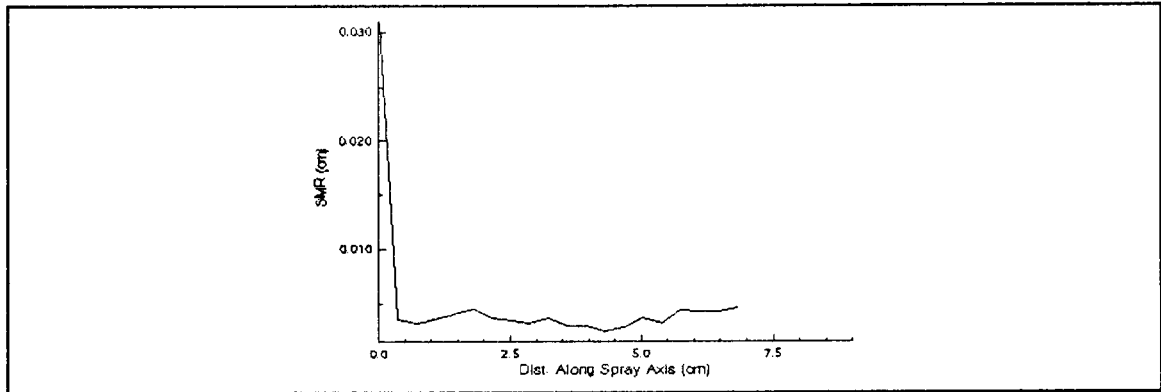


(b) 60 dgr. impingement; $v_{inj} = 1827$ cm/s

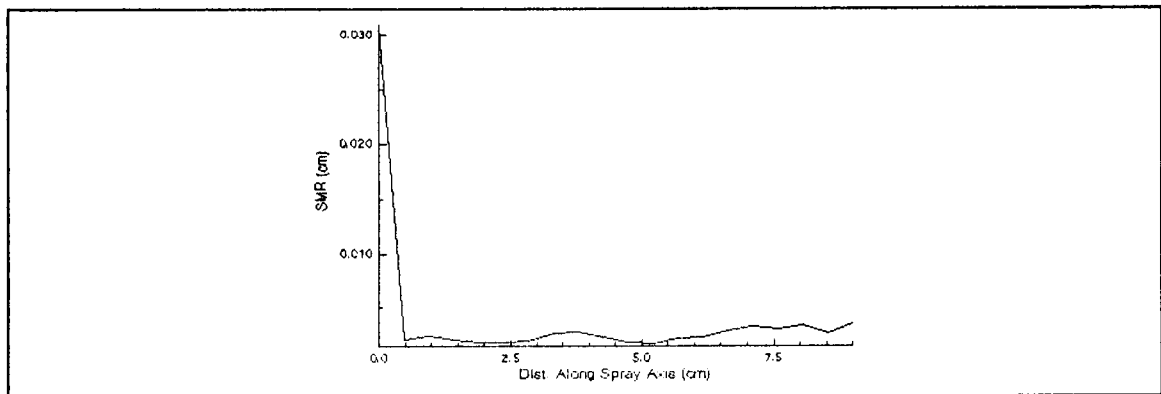


(c) 90 dgr. impingement; $v_{inj} = 1827$ cm/s

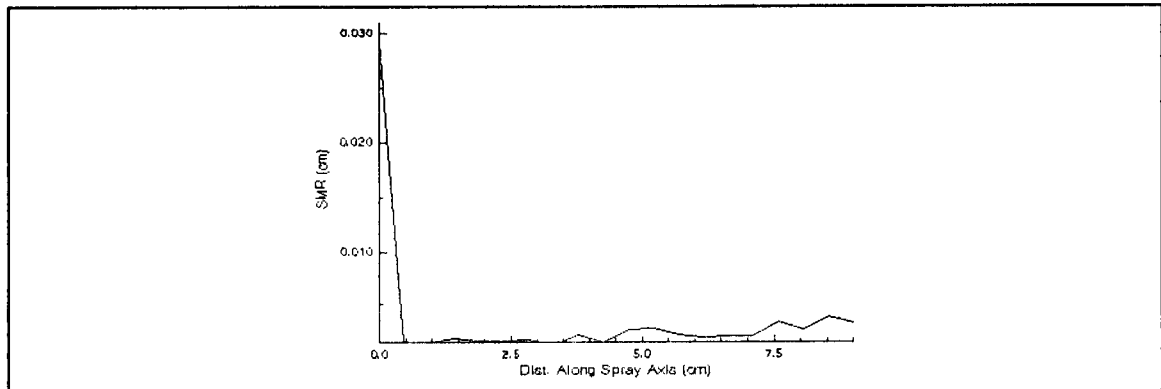
Figure 14. Computed SMR distribution along spray axis showing the effect of varying impingement angle.



(a) 60 dgr. impingement; $v_{inj} = 1218$ cm/s



(b) 60 dgr. impingement; $v_{inj} = 1827$ cm/s



(c) 60 dgr. impingement; $v_{inj} = 2436$ cm/s

Figure 15. Computed SMR distribution along spray axis showing the effect of varying injection velocity.

Figure 16 shows the computed distribution of gas axial and radial velocity components along the spray axis. Near the impingement point, the rapid rise in the gas velocity is due to entrainment of the gas by penetration of the liquid globules. The rate of increase of the gas velocity is affected by the rate of globule breakup. As the size of a globule decreases, its interaction with the gas is magnified due to the increase in globule acceleration. Note that the peak gas velocity is about one-half of the globule injection velocity indicating significant drag on a globule. Similar results occur for all of the cases considered.

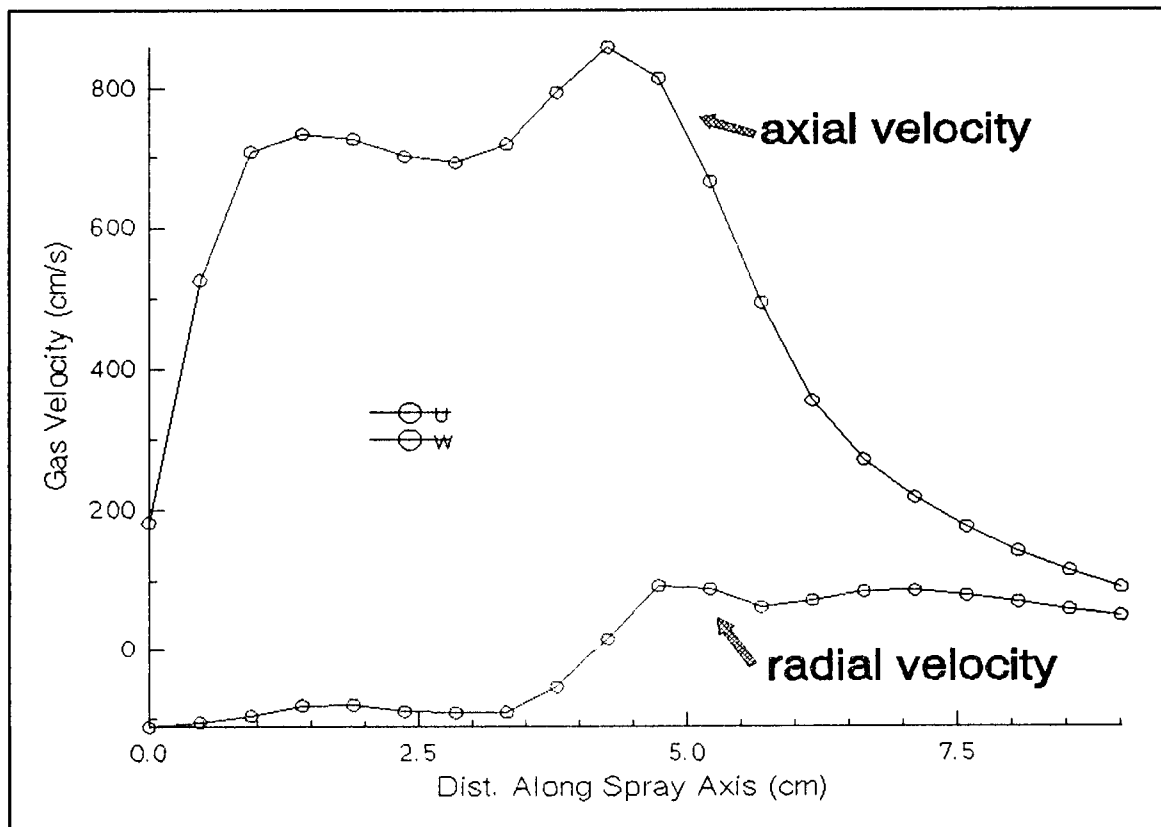


Figure 16. Computed gas axial and radial velocity components along spray axis for 60 dgr. impingement and $v_{inj} = 1827$ cm/s.

Unlike-doublet stream impingement

The second case of stream impingement considered consists of the impingement of liquid N_2H_4 and N_2O_4 via an unlike-doublet injector. An axisymmetric configuration was discretized and is illustrated in Figure 17 with 24 radial and 40 axial computational cells. A non-uniform mesh distribution was employed near the bounding wall in order to properly resolve the local velocity gradients. The domain consists of a cylindrical chamber with an outflow boundary where the pressure was specified to be 1 atm. Conditions for this simulation are given in Table II. Two impingement angles (90 dgr. and 60 dgr.) were computed to appraise the effect of stream impingement angle on the spray structure and also on the spray/wall interactions. Reactive stream impingement effects (blowapart) are insignificant for the present configuration based upon the criteria of Kushida and Houseman⁵.

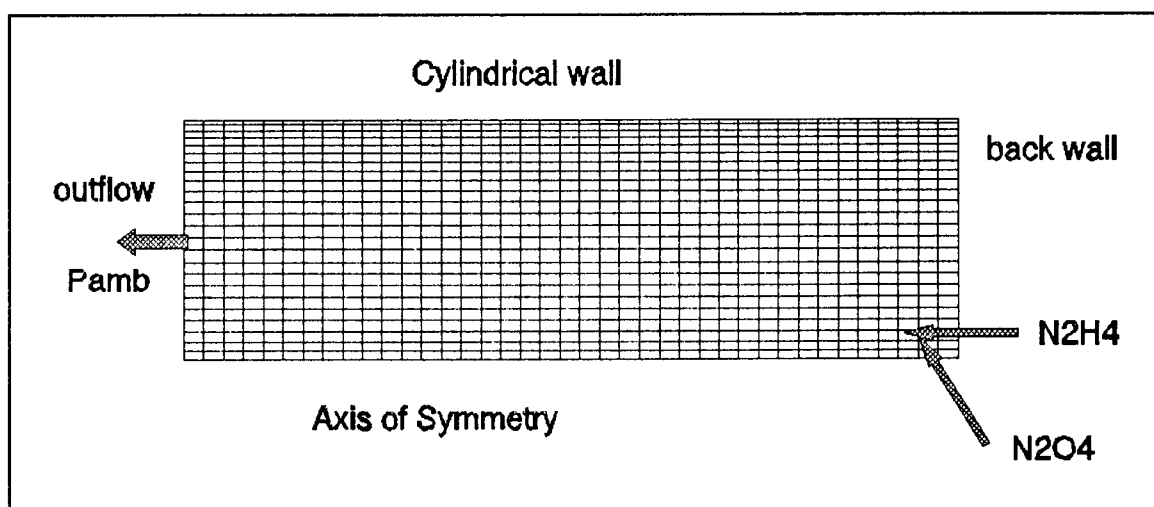


Figure 17. Computational domain for unlike-doublet stream impingement.

Table II. Conditions for N₂H₄/N₂O₄ unlike-doublet stream impingement.

Total Propellant Mass Flow, 13.83 g/s

N ₂ H ₄ Injection Velocity, 1950 cm/s axial

N ₂ O ₄ Injection Velocity, 1619 cm/s at 60 dgr. and 90 dgr. from axial

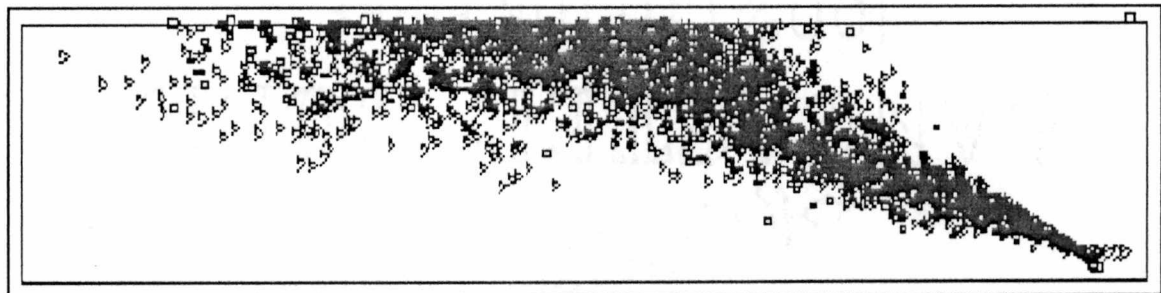
Fuel/Oxidizer ratio (F/O), .83; Momentum Ratio (F/O), 1.; Inj. Temp., 300 K

Chamber Diameter, 6 cm; Chamber Length, 10 cm; Orifice Diameter, .064 cm

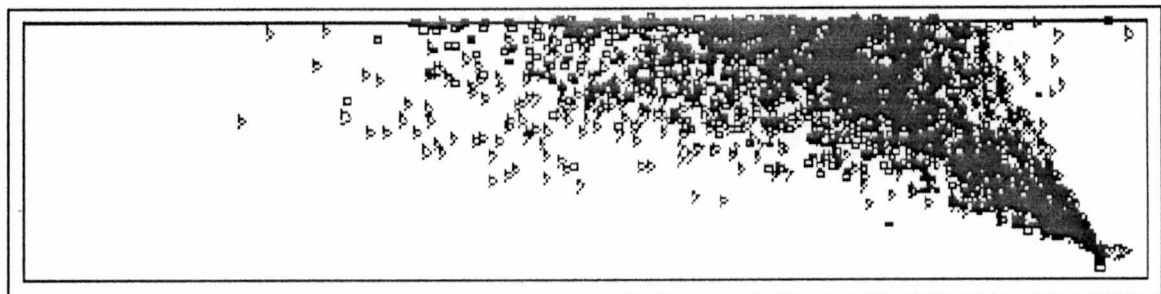
Figure 18 depicts the computed spray structure for the 90 and 60 degree impingements. N₂H₄ and N₂O₄ parcels are shown respectively as rectangles and triangles. Note that the two streams are well mixed with a momentum ratio of one. Both N₂H₄ (triangles) and N₂O₄ (rectangles) droplets impinge on the wall. There exist a complex combination of globule rebounding and tangential liquid jet flow at the wall. The computed spray velocity fields are shown in Figures 19 and 20. Note that the sprays are deflected downstream by the wall impingement action. A small amount of liquid back-splash is observed for the 90 degree impingement.

The majority of the N₂H₄ globules are observed to rebound after hitting the wall whereas those of the N₂O₄ spray tend to glide along the wall. These two different spray/wall interactions can be explained by the fact that the N₂H₄ surface tension (75 dynes/cm) being much larger than that of N₂O₄ (28 dyne/cm) results in a higher impact Weber number for the N₂O₄ globules. The N₂O₄

impact Weber number is probably higher than the critical value (50) separating the wall rebounding regime from the liquid jet flow. Thus, the majority of the N₂O₄ globules find themselves in the liquid wall jet regime.



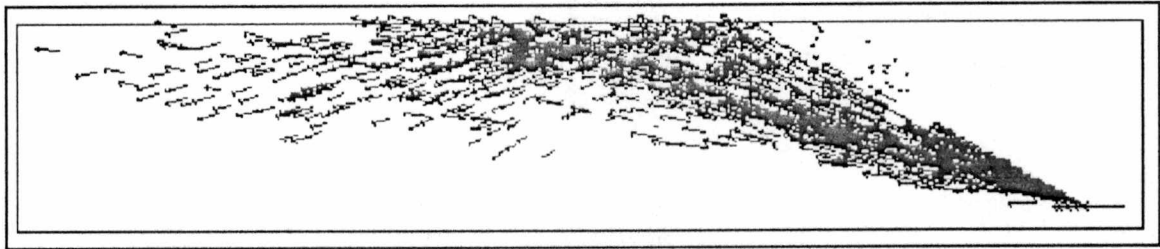
(a) 60 dgr. impingement



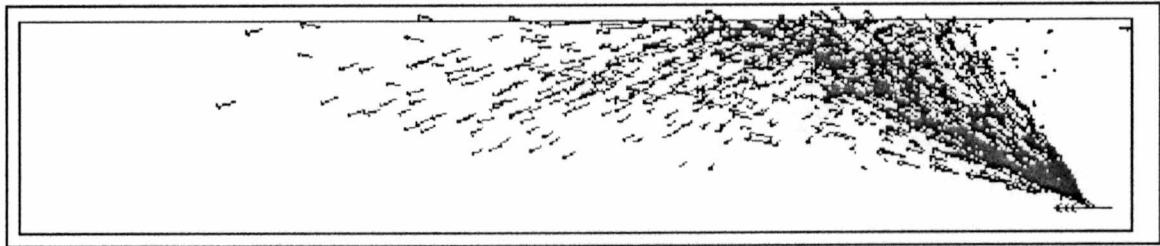
(b) 90 dgr. impingement

Figure 18. Computed N₂H₄/N₂O₄ unlike-doublet spray parcel trajectories illustrating the effect of impingement angle.

The 90 degree impingement results in wider spray dispersion (higher cone angle) than the 60 degree case. SMR distributions along the spray axis are shown in Figure 21 for the N₂H₄ spray. The level of spray equilibrium sizes are in accord with the correlation of Dickerson. It is observed that for the 90 degree impingement, the SMR distribution increases as the wall is approached. This is probably due to coalescence created by the high concentration of globules

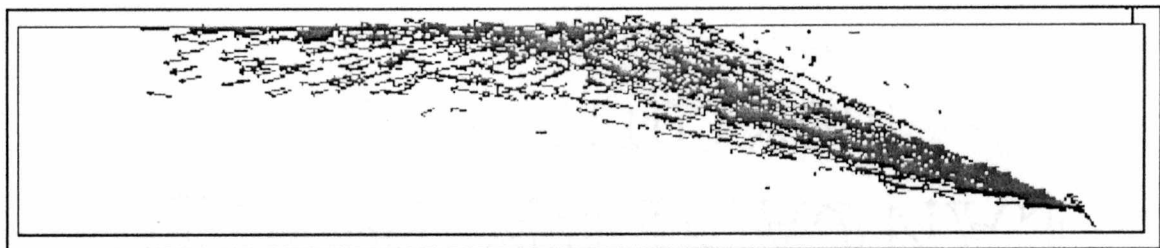


(a) 60 dgr. impingement

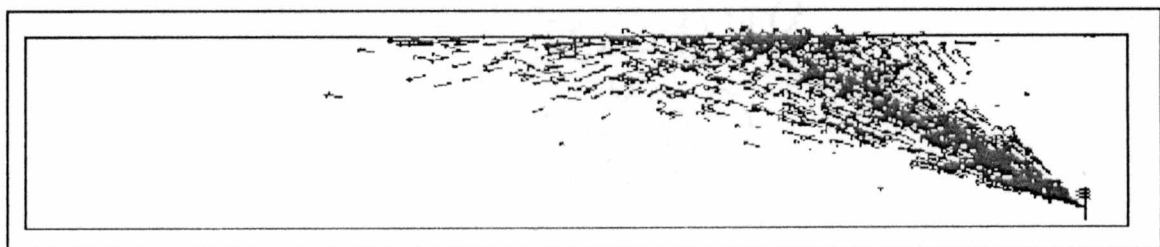


(b) 90 dgr. impingement

Figure 19. Computed N2H4 spray parcel velocity field for N2H4/N2O4 unlike-doublet simulation with varying impingement angle.

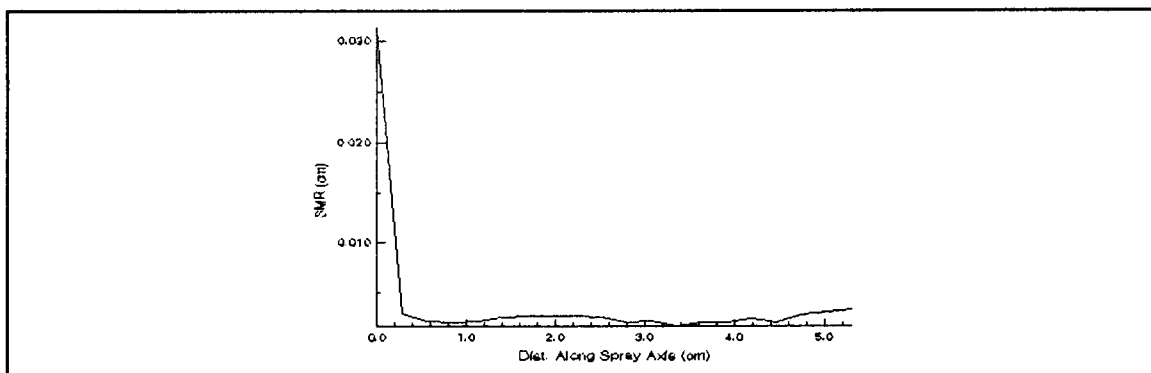


(a) 60 dgr. impingement

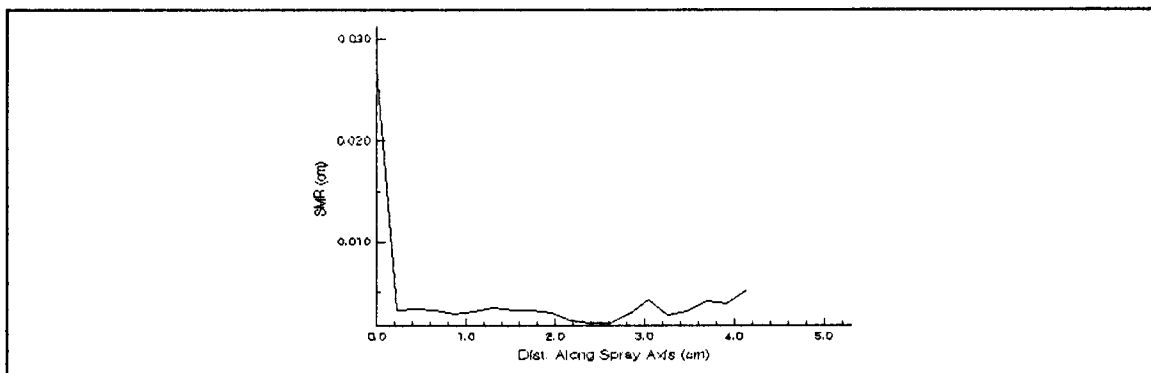


(b) 90 dgr. impingement

Figure 20. Computed N2O4 spray parcel velocity field for N2H4/N2O4 unlike-doublet simulation with varying impingement angle.



(a) 60 dgr. impingement



(b) 90 dgr. impingement

Figure 21. Computed N_2H_4 SMR distribution along spray axis for N_2H_4/N_2O_4 unlike-doublet simulation with varying impingement angle.

existing at the wall. Similar results are obtained for the N_2O_4 spray.

Gas velocity fields for the two impingement angles are depicted in Figure 22. The flow field is dominated by a large recirculation zone similar to that in a backward facing step. The 60 degree impingement induces a stronger gas velocity field in comparison to the 90 degree case. This is expected because of the longer spray penetration path available with the 60 degree impingement. Close examination of the downstream velocity distribution reveals a wall jet flowing downstream from the spray/wall impingement site. A small well-defined

recirculation eddy is observed in the 60 degree case. There is no definitive evidence of drop entrainment by either the large recirculation zone or the small recirculation eddy.

The impinged liquid imparts a tangential momentum component to the gas in the immediate vicinity of the wall through the action of drag. This is evident in the 90 degree case by the slightly higher velocity near the wall following impingement. It is this spray/wall momentum exchange that is responsible for the creation of a wall jet in the gas moving tangent to the wall away from the impingement site.

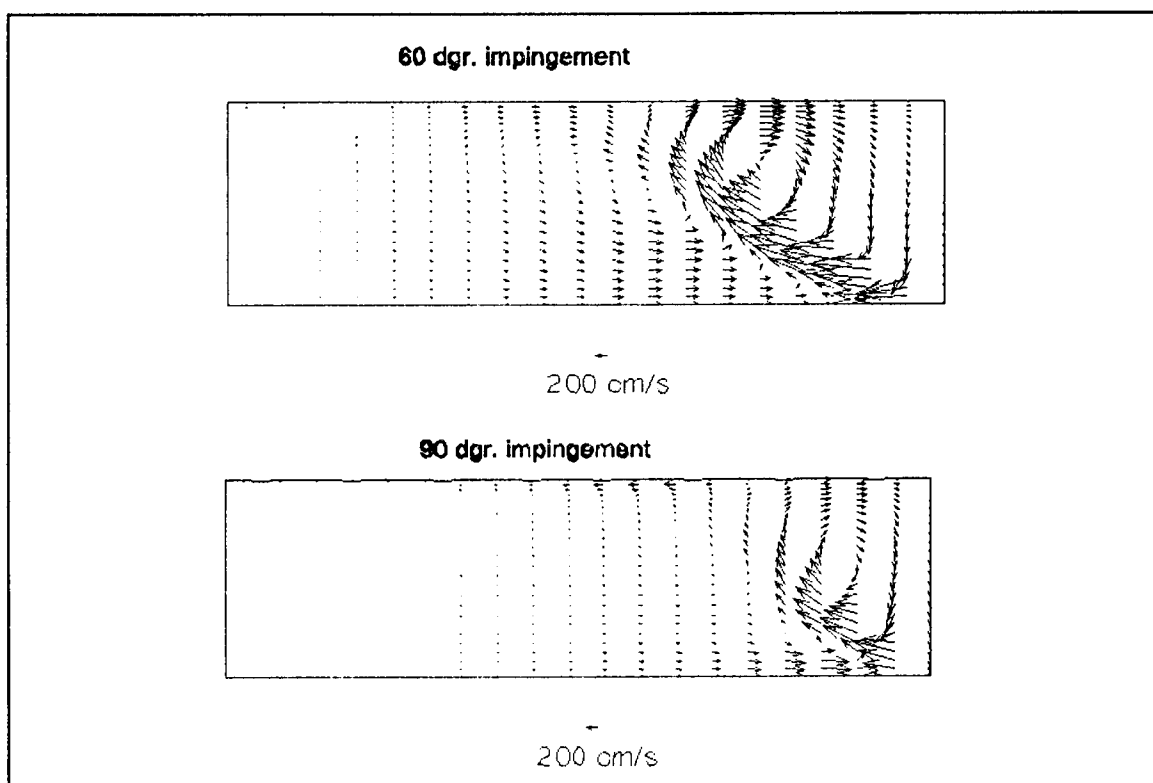


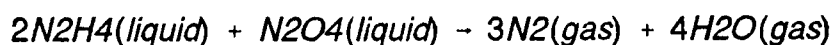
Figure 22. Computed gas velocity vectors for N₂H₄/N₂O₄ unlike-doublet simulation with varying impingement angles.

5.2 Bipropellant Spray Combustion via Unlike-Doublet Impingement

This section presents results of a simulation of the combustion of a spray produced by impinging two cylindrical unlike-liquid streams. Exactly the same axisymmetric configuration as illustrated in Figure 17 was employed. Two different bipropellant systems (N₂H₄/N₂O₄ and N₂H₄/LOX) were computed to illustrate the effect of propellant combinations. The initial gas flow field consisted of a quiescent N₂ gas at a pressure of 7 atm and a temperature of 600 K. This initial temperature was selected in order to reduce the transient ignition period. A 90 degree impingement angle was used with all other parameters being exactly the same as those in Table II.

N₂H₄/N₂O₄ bipropellant spray combustion

The N₂H₄ liquid fuel is directed axially with an initial temperature of 300 K and is forced to impinge with a radially directed N₂O₄ liquid oxidizer at this same initial temperature. A maximum heat release rate of 83,000 kcal/(sec)(mole of N₂O₄) was estimated for the liquid interfacial reactions produced by this hypergolic propellant combination. The liquid phase reaction was assumed to be:



with the reaction constants B and E_a being respectively 6.75E15 (cc/mole/s) and 1.3E4 K. These values are taken from Sawyer⁵⁴ for gas phase reactions of the N₂H₄/N₂O₄ system.

N₂O₄ decomposes very rapidly to NO₂ in the gas phase. The approximation that NO₂ is the vaporizing gaseous specie was thus made for the N₂O₄ liquid oxidizer. Using this approximation, it was possible to account for chemical change by adding the heat of decomposition to the heat of vaporization for N₂O₄. The gas phase decompositions of N₂H₄ and NO₂ were ignored because their reaction rates are much slower than those of the oxidation reactions. A bipropellant envelope flame droplet combustion model was employed for both fuel and oxidizer droplets. The chemical scheme adopted is shown in Table III. This scheme is an adaptation of a more detailed one described by Sawyer. Arrhenius kinetic rate parameters were obtained from Sawyer and the reaction rate was taken to be the minimum of that given by either the kinetic rate or the turbulent mixing-controlled rate ($A_1 = 16$). An equilibrium chemistry was also employed to account for high temperature (above 3000 K) dissociations. The equivalence ratio for this simulation is 1.193 (i.e., fuel rich).

Table III. Gas chemistry for N₂H₄/N₂O₄ system.

Kinetic Reactions

N ₂ H ₄ + 2NO ₂ -> 2H ₂ O + 2NO + N ₂
N ₂ H ₄ + 2NO -> 2H ₂ O + 2N ₂

Equilibrium Reactions (above 3000 K)

2H ₂ O -> 2H ₂ + O ₂
N ₂ -> 2N

Since the $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ combination is hypergolic (i.e., rapid oxidation), an artificial ignition procedure was not necessary to initiate combustion. The transient behavior of the combustion flow field was tracked in time until a pseudo-steady state was achieved (40-50 ms) with fixed boundary conditions. Figure 23 shows the temporal evolution of the liquid parcel trajectories. At $t=5$

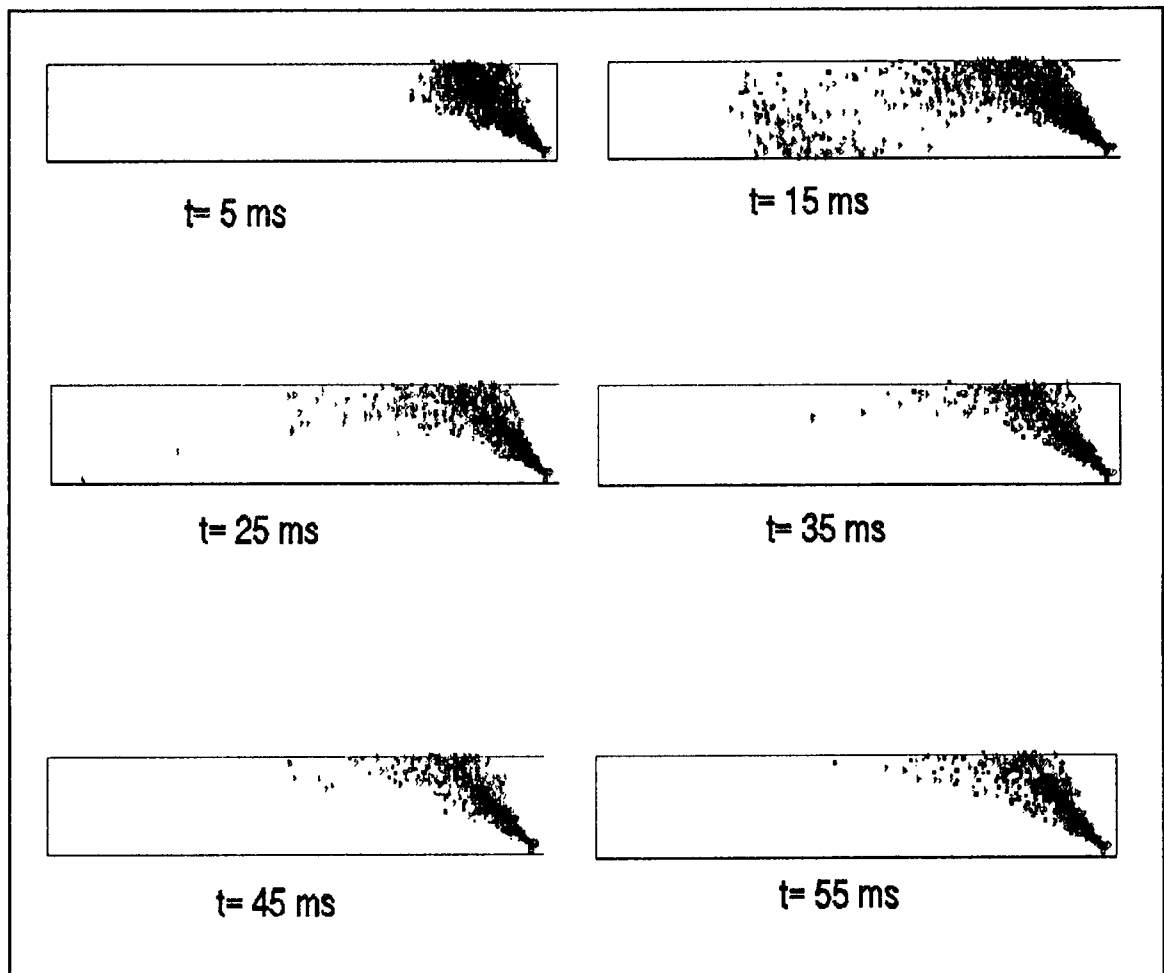


Figure 23. Computed spray structure for $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ spray combustion from an unlike-doublet.

ms, the spray has just reached the wall. Between $t=5$ ms and $t=15$ ms, the spray/wall interaction is at its peak with most of the globules which have strike

the wall rebounding towards the chamber axis. Thereafter, The spray vaporization process depletes the globule population until a pseudo-steady state is arrived at. It should be noted that both N_2H_4 (triangles) and N_2O_4 (rectangles) accumulate near or at the wall. This situation may be of concern for gas/wall compatibility.

The temporal evolution of the gas velocity field is depicted in Figure 24. The corresponding temperature field is shown in Figure 25. At $t=5\text{ms}$ a reaction zone mirroring the developing spray structure is observed. This zone consists of a relatively hot outer layer with a cool inner core where spray vaporization is prevalent. Hence at this early stage, the combustion process is greatly influenced by the atomization process and the ignition characteristics.

At later times, two recirculation regions are established near the impingement point. Combustion is initiated at the outer portion of the chamber and propagates towards the chamber axis. The outer recirculation zone close to the wall acts as a flame holder whereas the inner zone promotes mixing of the propellant vapors transported towards the chamber axis. This is evident in Figure 26 which shows the pseudo-steady state N_2H_4 and NO_2 species mass fractions.

An outer fuel rich region is observed along with an inner oxidizer rich zone. There appears to be an easily flammable band of fuel-oxidizer mixture along the spray axis near the impingement region. Fuel vapors penetrate the inner oxidizer

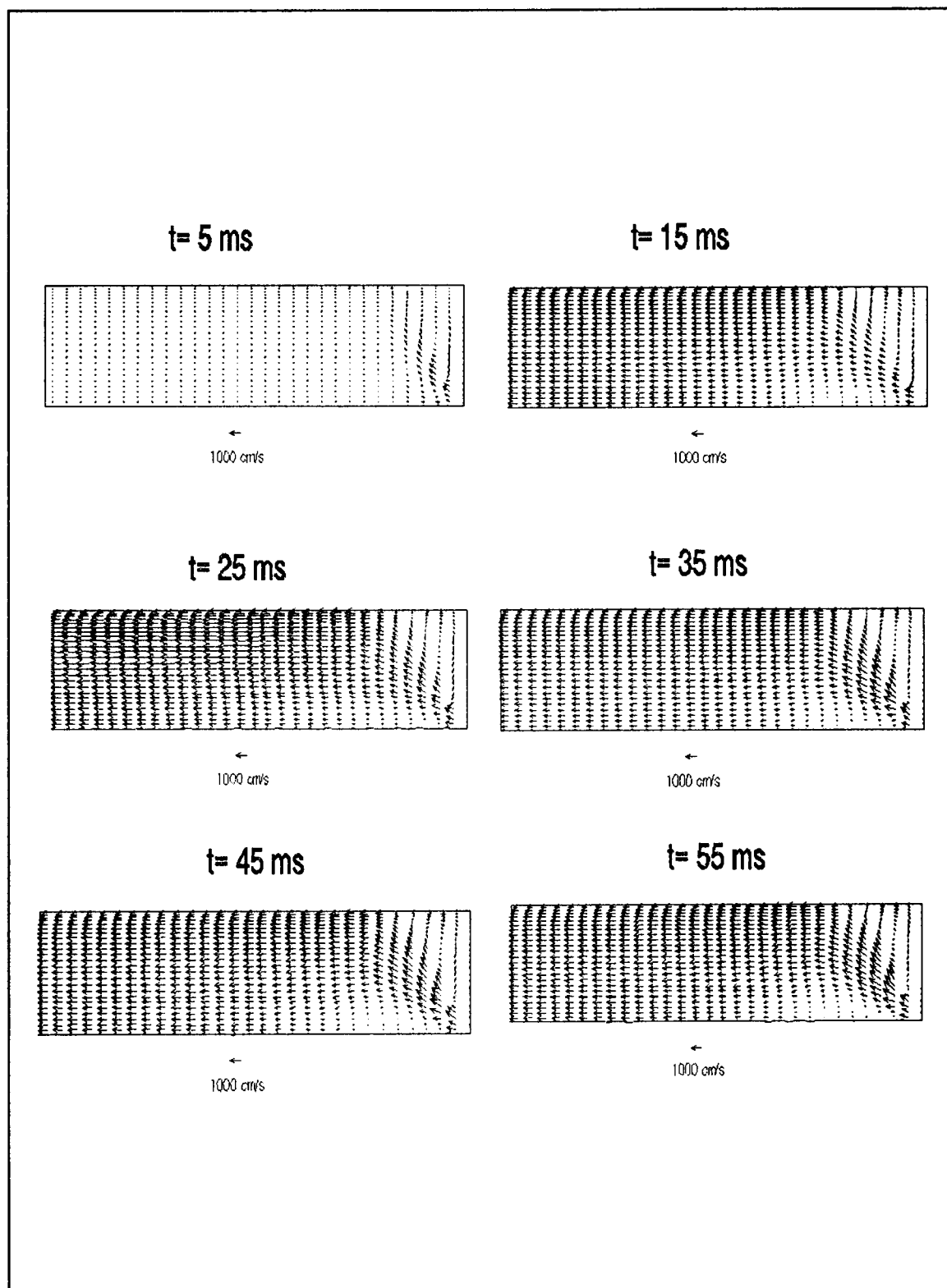


Figure 24. Computed temporal evolution of the gas velocity field for $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ spray combustion.

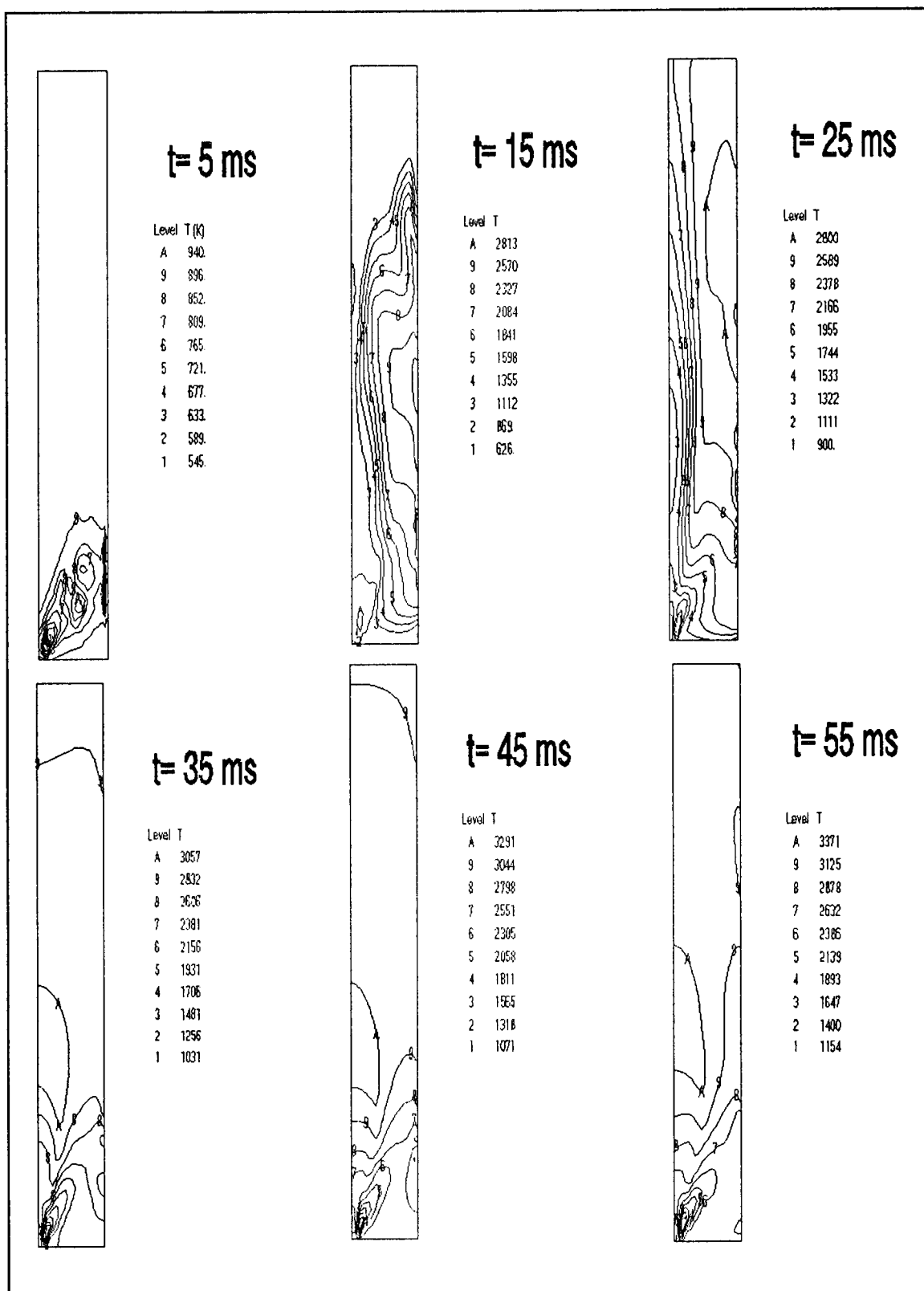


Figure 25. Computed gas temperature field for N₂H₄/N₂O₄ spray combustion.

region and are mixed by the action of the inner recirculation vortex. A well-mixed combustion flow field is established at the chamber exit. Figure 27 depicts the primary combustion product mass fractions illustrating the uniformity of the combustion process.

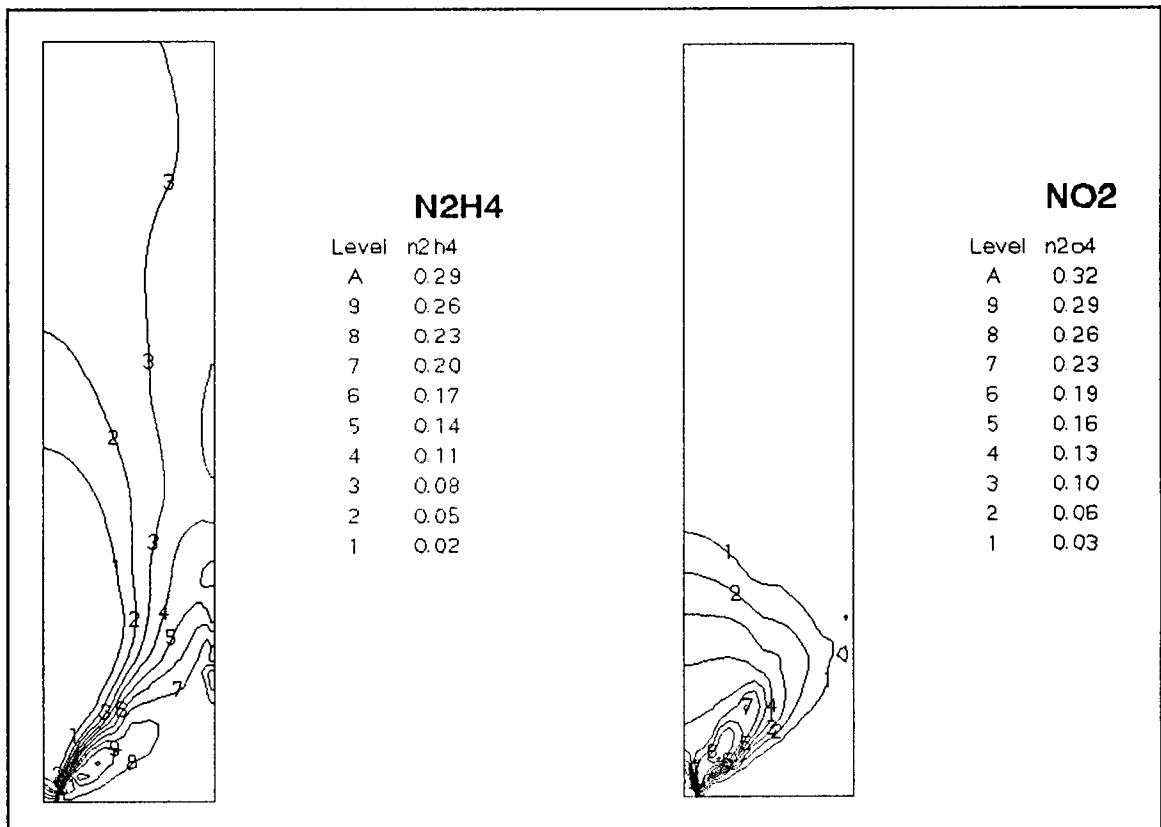


Figure 26. N₂H₄ and NO₂ species mass fractions for N₂H₄/N₂O₄ spray combustion.

The computed H₂O mass fraction profiles and temperature levels are similar to those observed by Burrows³ using an unlike-doublet injector. The configuration employed by Burrows had a larger orifice diameter (.175 cm) and operated at a higher combustion pressure (19 atm) than what is presented here.

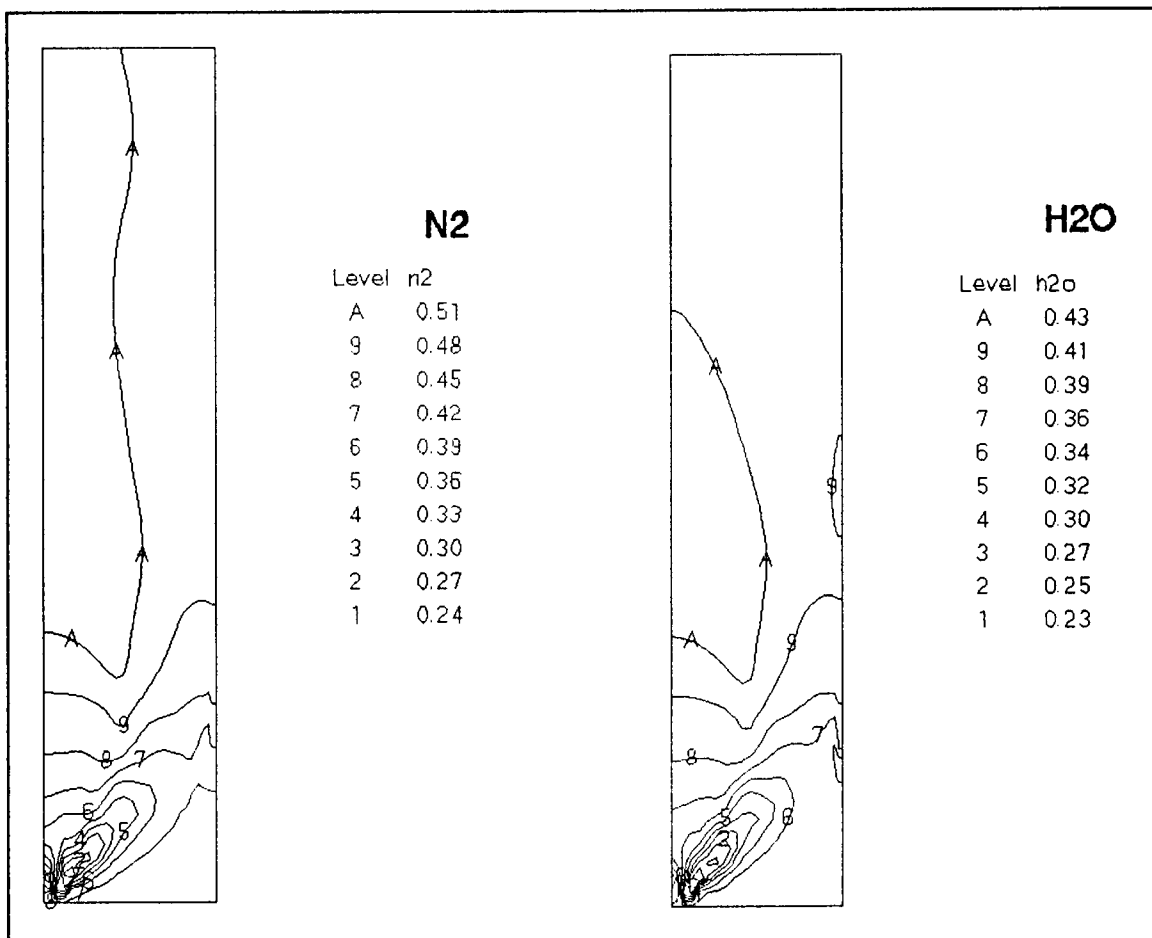


Figure 27. Computed mass fractions of the primary combustion products from N₂H₄/N₂O₄ spray combustion.

Burrows observed that the propellants were not very well-mixed due to reactive stream blowapart. The computed combustion field shows no evidence of reactive stream effects at a pressure of 7 atm. A computation at an elevated pressure was made in order to asses the effect of reactive stream impingement. Exactly the same configuration was employed except that the chamber back-pressure was set at 30 atm. The computed time history of the spray parcel trajectories for this high pressure case is shown in Figure 28.

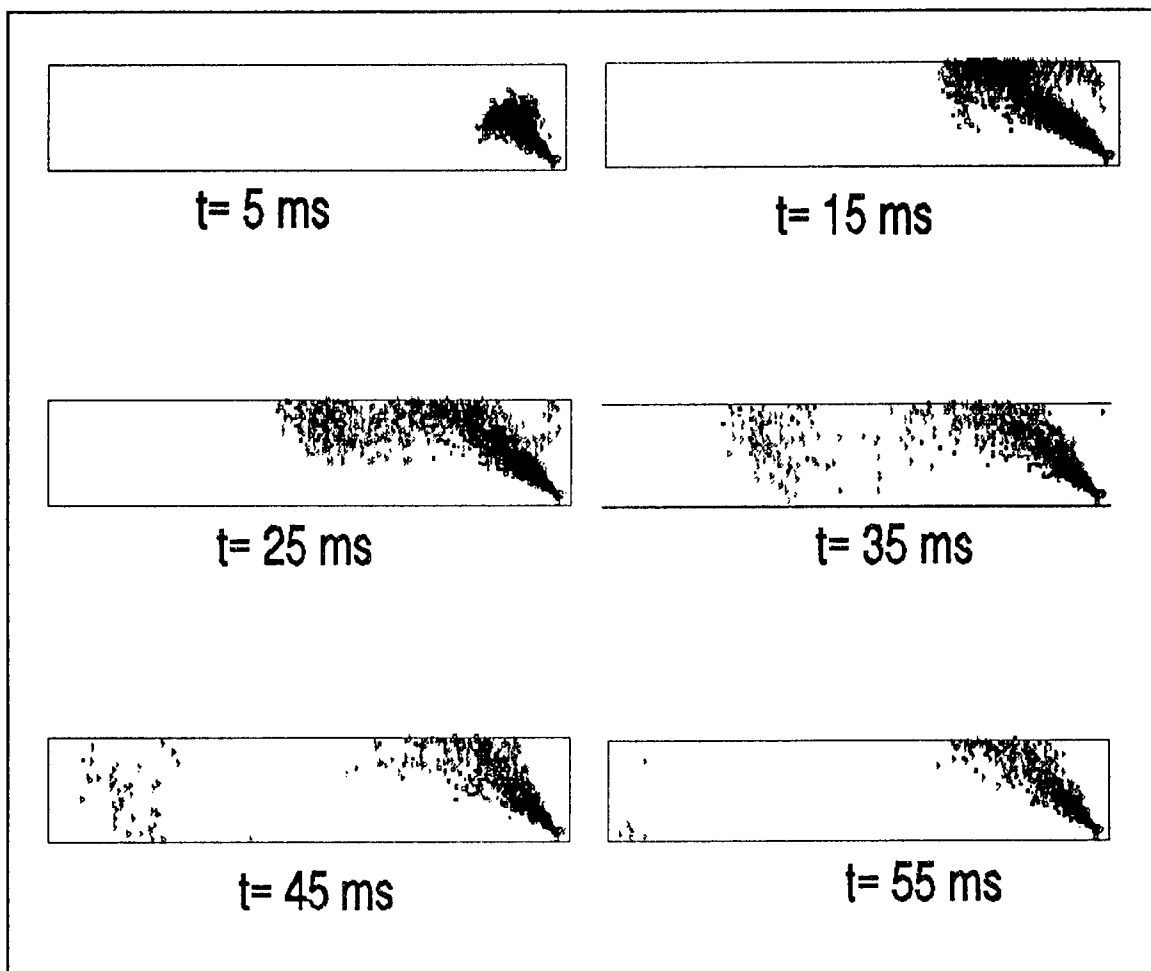


Figure 28. Computed spray structure for high pressure $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ spray combustion.

At this elevated pressure, the pressure potential tending to push the two streams away from each other is greater than at 7 atm. This results in a somewhat higher coefficient of restitution for globule impingement collision. The plots in Figure 28 show that at the early stages, the spray is not well-mixed. Some of the N_2H_4 globules are deflected in the direction of the back-wall. At later stages, the spray becomes more uniform but still not with the same mixing effectiveness as observed for the lower pressure case (Fig. 23). A pseudo-steady state has not been established yet.

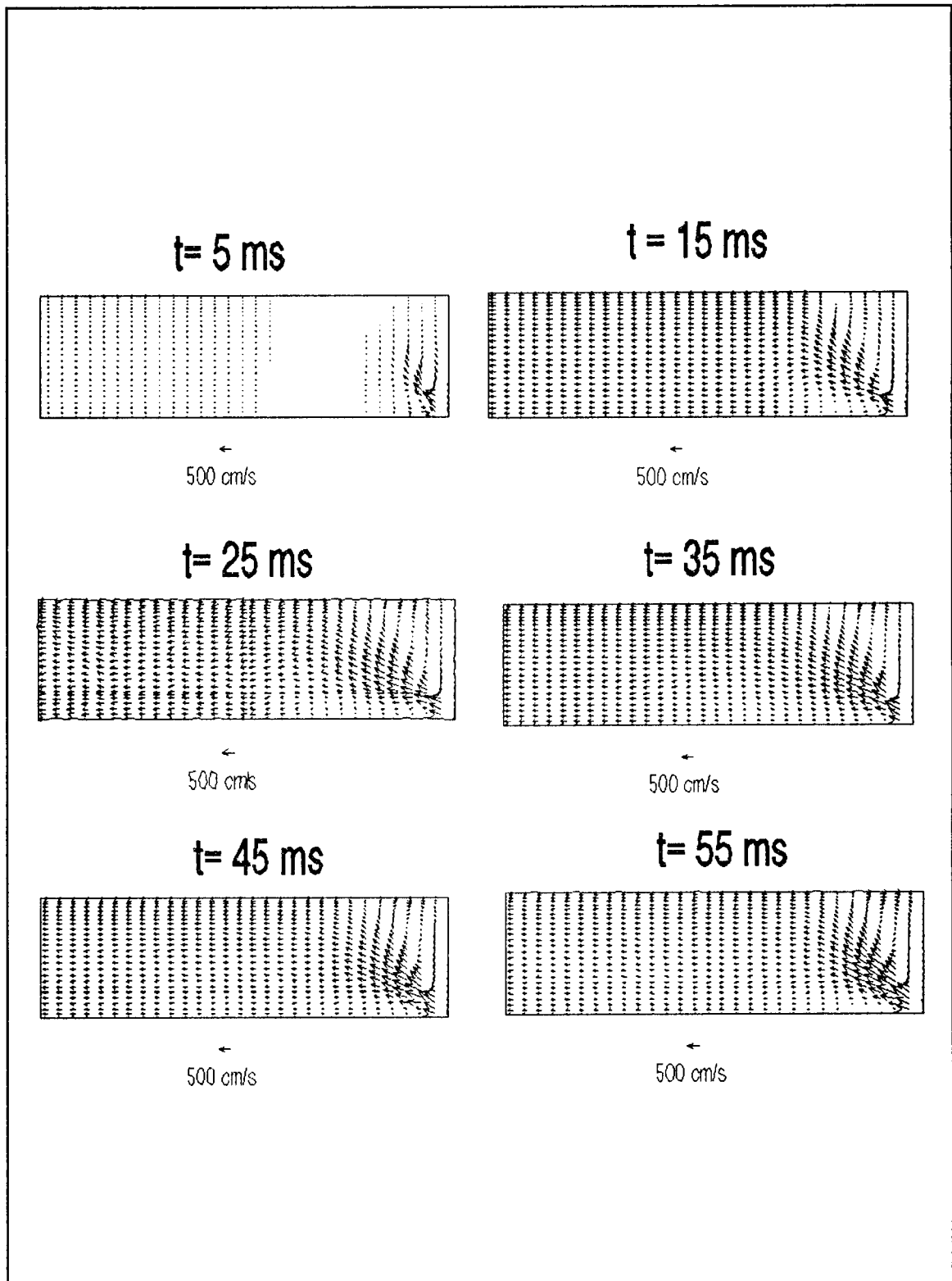


Figure 29. Computed gas velocity field for high pressure $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ spray combustion.

Figure 29 depicts the temporal evolution of the gas velocity field for the high pressure case. The structure of this velocity field is similar to that of the 7 atm case (Fig. 24). Differences are manifested in the lower velocity magnitudes. The recirculation strengths are seen to be much weaker, especially the inner eddy. As a result, the development of the combustion field (Fig. 30) is observed to be much slower and less uniform than the 7 atm case.

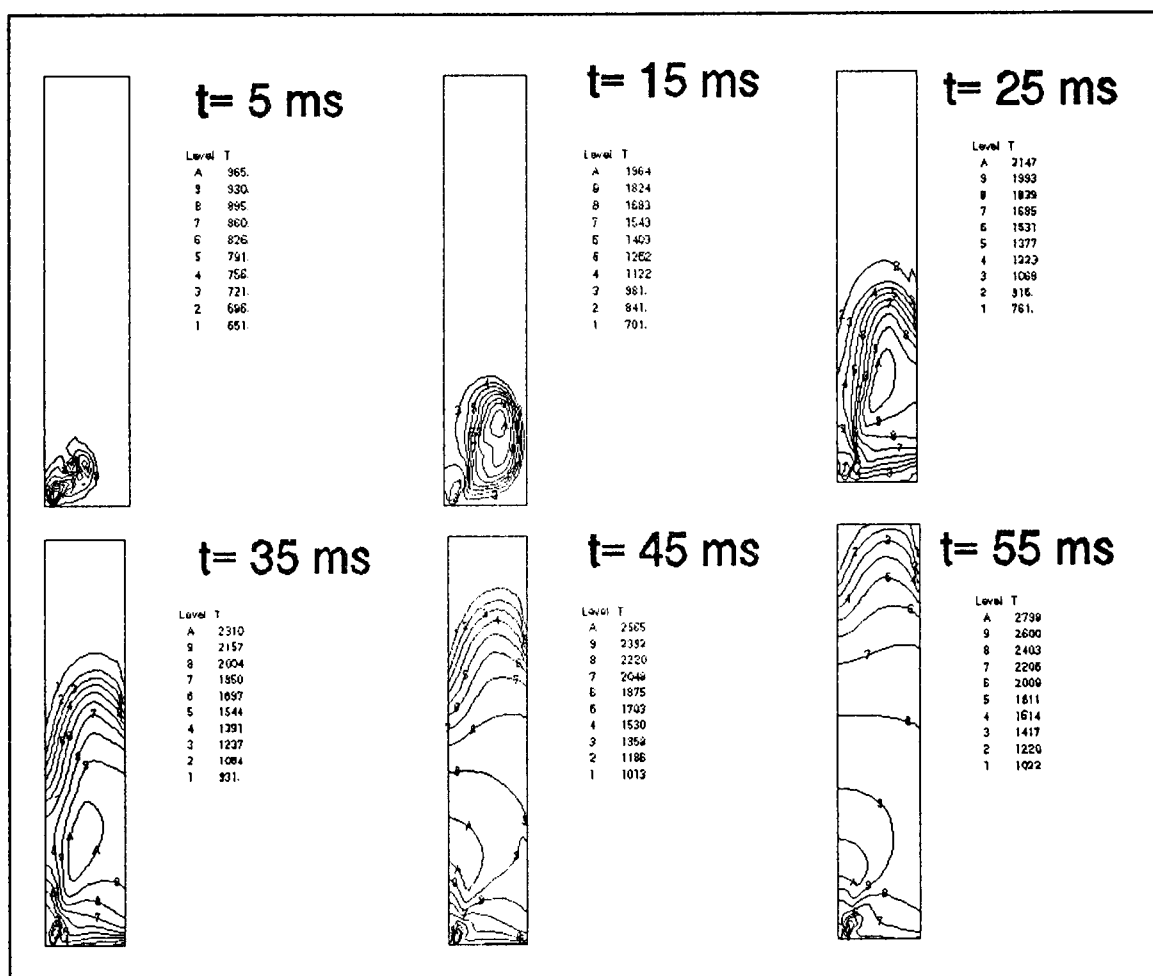


Figure 30. Computed gas temperature field for high pressure N_2H_4/N_2O_4 spray combustion.

The propellant gas mass fraction contours at $t=55\text{ms}$ are illustrated in Figure 31 for the high pressure case. It can be seen that the propellant vapors are more stratified than the 7 atm case. This results in the lower temperatures and velocities observed. Hence, reactive stream effects are detrimental at high pressures for this configuration.

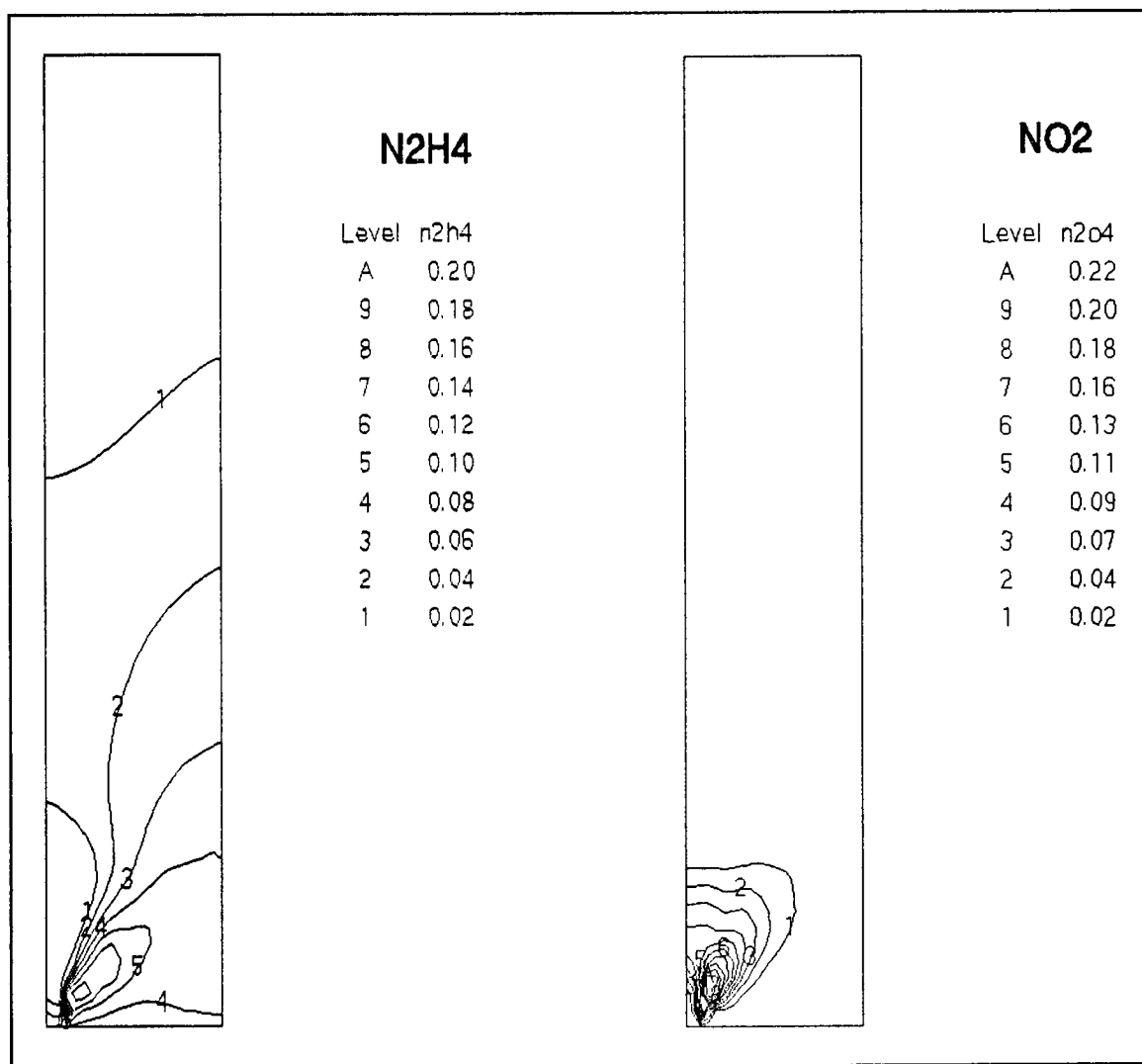


Figure 31. N₂H₄ and NO₂ gas mass fractions for high pressure N₂H₄/N₂O₄ spray combustion.

N₂H₄/LOX bipropellant spray combustion

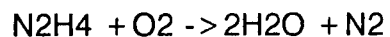
For this simulation, the N₂O₄ oxidizer was replaced with liquid oxygen (LOX) directed radially with an initial temperature of 104 K. Note that the boiling point of LOX is considerably lower than that of N₂O₄. The gas phase decomposition of N₂H₄ was included in this case because the decomposition reaction rate is comparable to that of oxidation. This necessitated the use of a decomposition flame model for the N₂H₄ droplet combustion. A bipropellant envelope flame droplet combustion model was employed for the LOX oxidizer droplets. The chemical scheme adopted is given in Table IV. Again, the Arrhenius kinetic rate parameters were obtained from Sawyer and the reaction rate was taken to be the minimum of that given by either the kinetic rate or the turbulent mixing-controlled rate. At temperatures above 3000 K, an equilibrium chemistry was also employed to account for dissociations. The equivalence ratio for this case is .83 (i.e., oxidizer rich). Since this propellant combination is not hypergolic, an ignition source of 5 ms duration was employed to initiate combustion.

Figure 32 shows the temporal evolution of the computed spray structure. It can be seen that the time period to achieve a pseudo-steady state is less than that of the N₂H₄/N₂O₄ combination. The surface tension of LOX is smaller than that of N₂O₄. This smaller surface tension results in a slightly smaller drop size for the LOX spray. There doesn't appear to be any LOX droplets (rectangles) on the wall. All of the LOX spray is vaporized close to the impingement point. Hence,

the N₂H₄/LOX combination is similar to a liquid N₂H₄ spray in a gaseous O₂ environment.

Table IV. Gas chemistry For N₂H₄/O₂ system.

Kinetic Reactions



Equilibrium Reactions (above 3000 K)

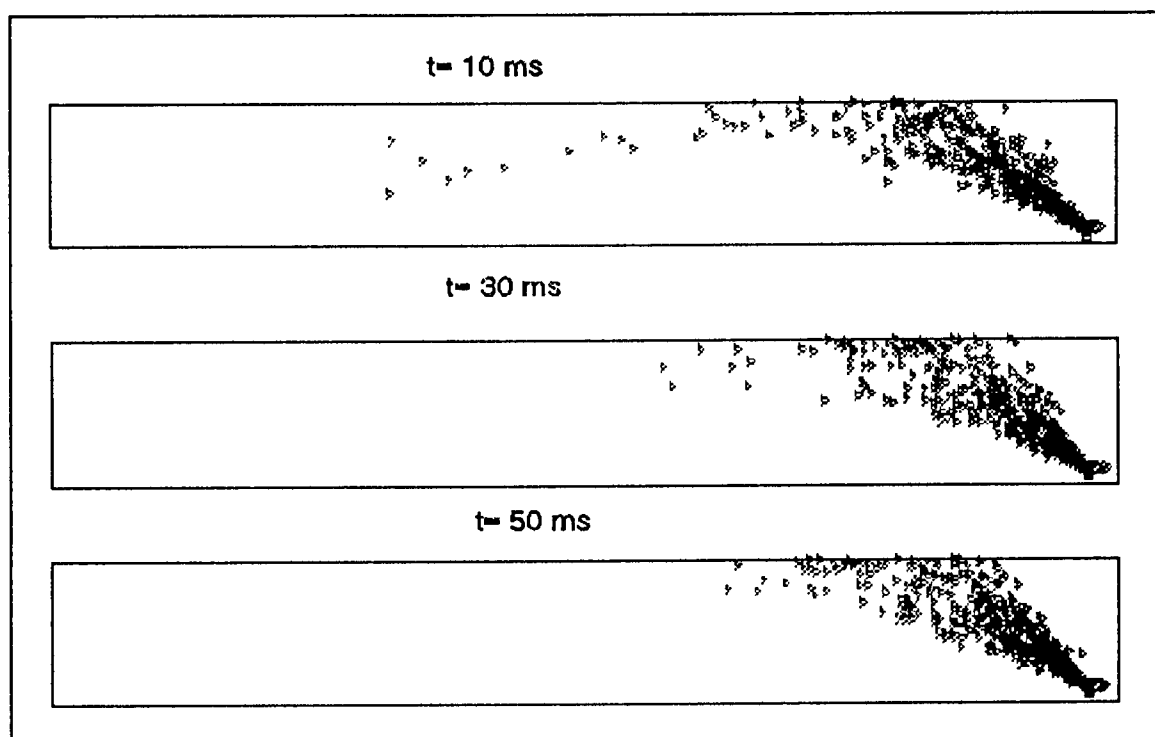
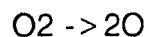
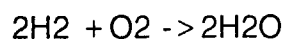


Figure 32. Computed spray structure for N₂H₄/LOX spray combustion from an unlike-doublet.

The computed gas velocity field is depicted in Figure 33 for different transient stages. Not much significant changes are observed in the evolution of the velocity field. This field is primarily unidirectional except for a small volumetric expansion region near the point of injection. The gas temperature field is shown in Figure 34.

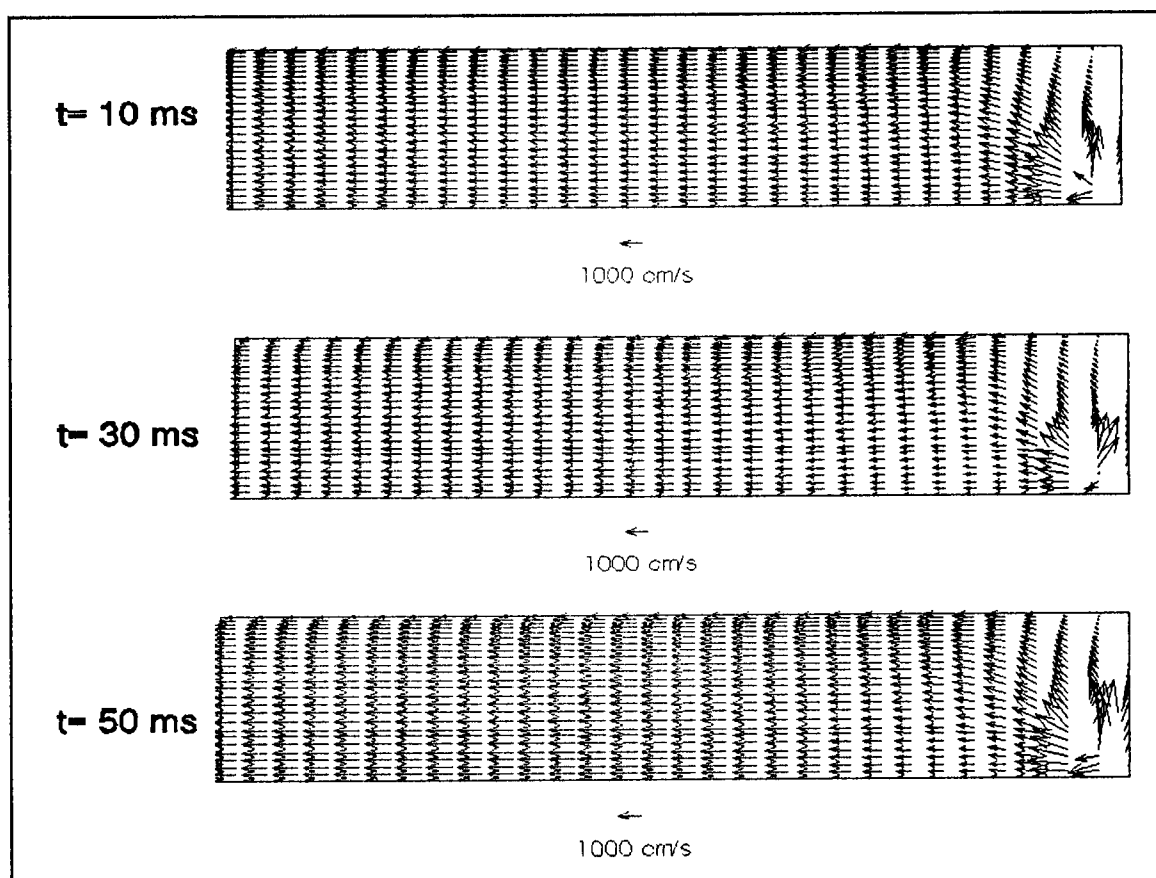


Figure 33. Computed gas velocity field for N₂H₄/LOX spray combustion.

A rapid combustion zone is established near the point of impingement causing the gas volume to undergo large expansion rates. It is observed that the combustion characteristics of the N₂H₄/LOX combination are vastly different

from those of the $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ combination. The $\text{N}_2\text{H}_4/\text{LOX}$ flame front proceeds axially and engulfs the entire chamber volume whereas that of the $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ combination proceeds along the spray axis and is transported inward by the spray/gas flow interactions. Hence, the $\text{N}_2\text{H}_4/\text{N}_2\text{O}_4$ combustion is mixing-controlled whereas that of $\text{N}_2\text{H}_4/\text{LOX}$ is vaporization controlled.

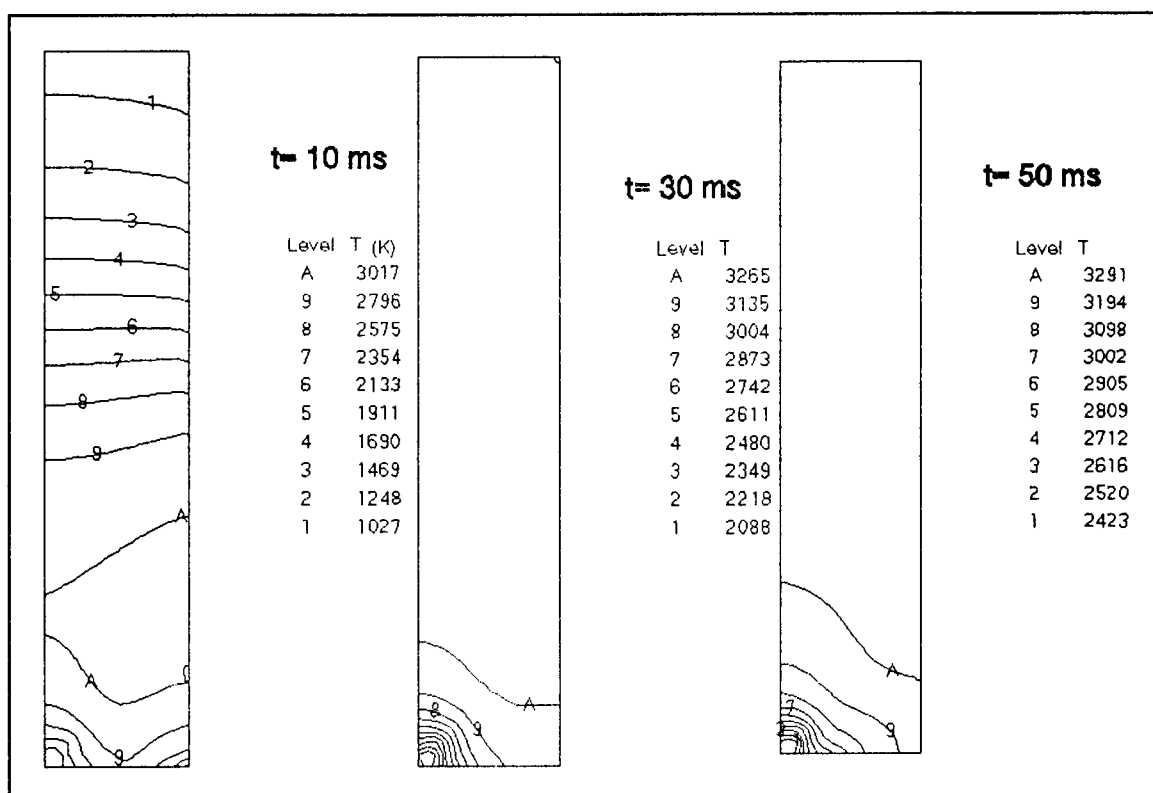


Figure 34. Computed gas temperature field for $\text{N}_2\text{H}_4/\text{LOX}$ spray combustion.

The N_2H_4 and O_2 mass fractions at a pseudo-steady state are presented in Figure 35. Note that virtually all of the N_2H_4 fuel is consumed near the impingement point. The O_2 vapors penetrate the entire chamber cross-section before being consumed. Figure 36 shows the corresponding mass fractions of

the primary combustion products (N_2 and H_2O). A very uniform combustion flow structure is produced at the exit of the chamber.

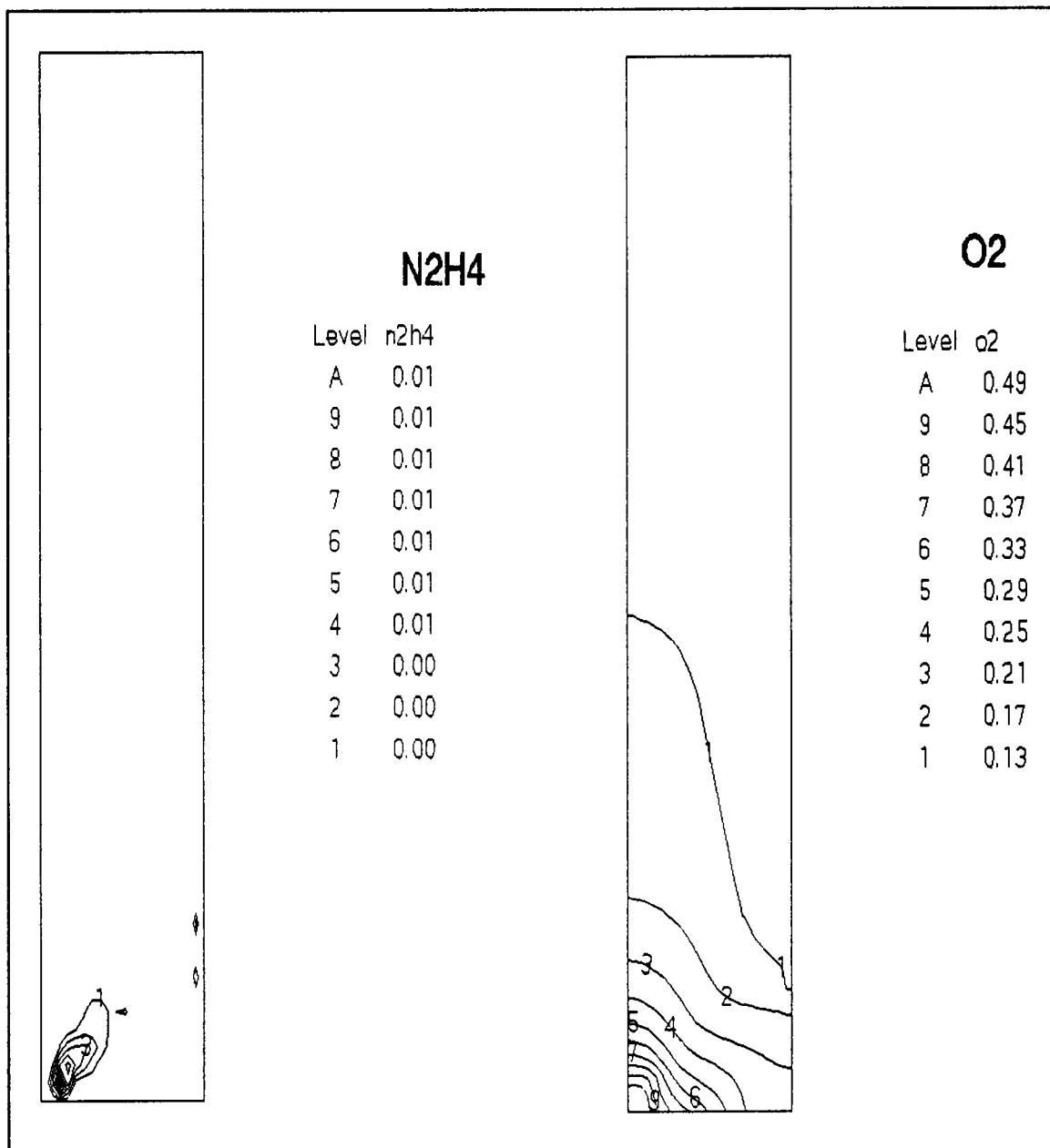


Figure 35. Computed N_2H_4 and O_2 mass fractions for N_2H_4/LOX spray combustion.

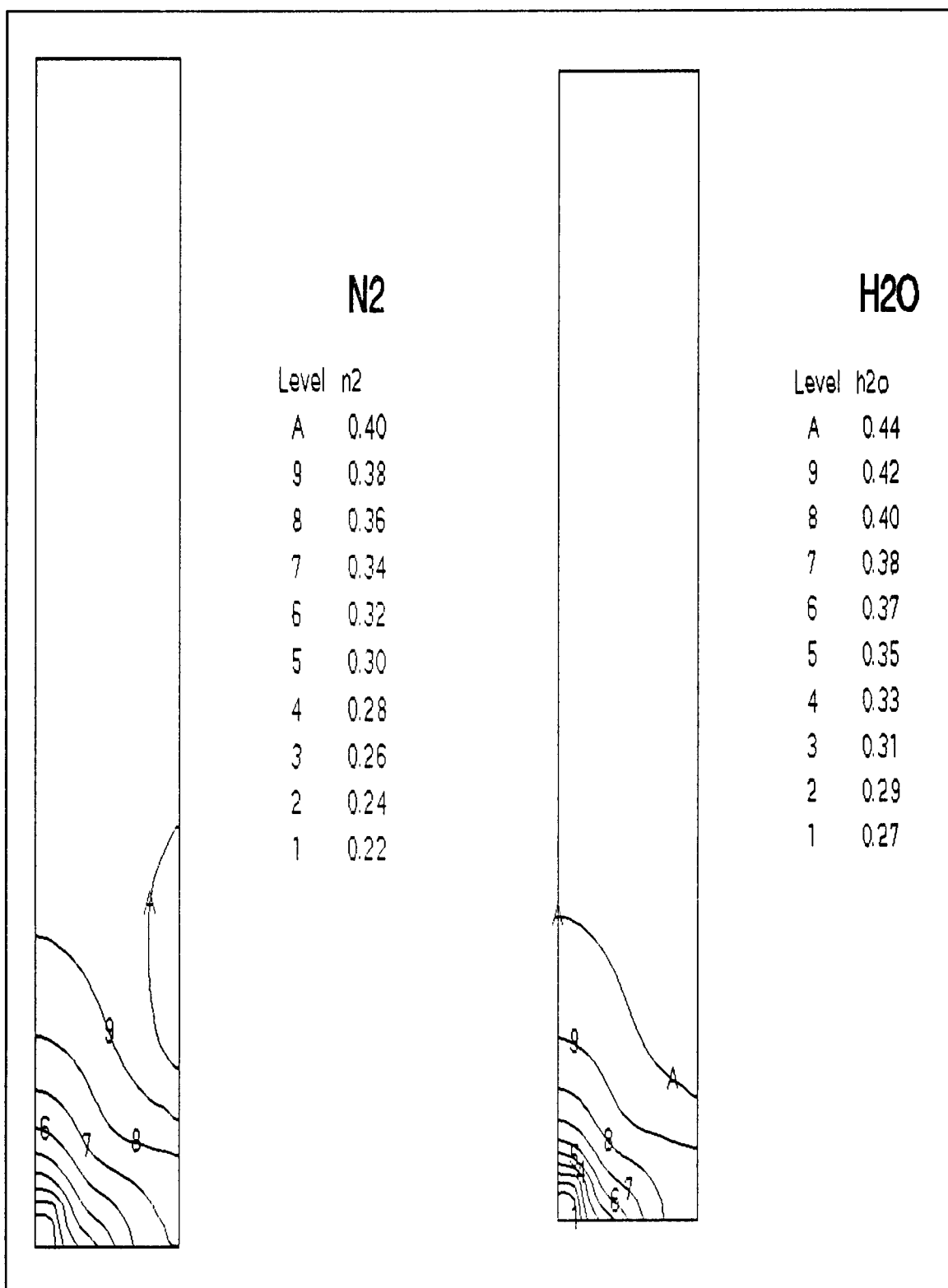


Figure 36. Computed primary combustion product mass fractions for N₂H₄/LOX spray combustion.

5.3 N₂H₄/LOX Spray Combustion in a VTE

The variable thrust engine (VTE) designed by TRW for the Orbital Maneuvering Vehicle (OMV) employs a single-element coaxial pintle injector with low propellant mixture ratio to address combustion gas/wall compatibility concerns. This injector is intended to achieve the particular impingement of the fuel spray on the wall without any significant oxidizer droplet accumulations. A simulation of this combustor employing the bipropellant combination N₂H₄/LOX is presented in this section.

The single-element pintle coaxial injector consists of an annular sheet of axially directed LOX oxidizer impinging upon N₂H₄ fuel streams injected radially outward from a series of uniformly spaced slots. Performance is controlled through fuel slot sizing as well as oxidizer sheet thickness. An axisymmetric cylindrical configuration was assumed for this simulation. The pintle injector was modeled by injecting LOX globules with a radius equal to the annulus height of the oxidizer port and fuel globules with an effective circular radius reflecting the flow area of a slot element. Parameters for this simulation are given in Table V. An axisymmetric mesh consisting of 24 radial and 60 axial computational cells was employed. The computations were initiated by introducing bipropellant globules within a quiescent chamber at a temperature of 400 K and a pressure of 11 atm. An ignition source of 5 ms duration was activated at 4 cells down-

stream of impingement.

Table V. Conditions for N₂H₄/LOX spray combustion in a VTE.

Mass Flow, 261 g/s; Mixture Ratio (O/F), .72; Chamb. Dia., 6.2 cm; Chamb. Length, 14 cm					
$V_{inj,fu}$ (cm/s)	$V_{inj,ox}$ (cm/s)	D_{fu} (cm)	D_{ox} (cm)	T_{fu} (K)	T_{ox} (K)
2311	1824	.055	.062	300	104

A decomposition flame model was employed for the N₂H₄ droplet combustion along with a bipropellant envelope flame model for the LOX droplets. The same chemical scheme as given in Table IV was used. A pseudo-steady state was achieved at about a time of 50 ms after injection. Results are presented for this pseudo-steady state only.

The spray trajectory is depicted in Figure 37. It is observed that a very thin spray is produced with N₂H₄ droplets (triangles) impinging on the wall. The LOX droplets are completely vaporized before reaching the wall. A reason for the spray being thin is that because of the high liquid mass flow rate, the globule number concentration is high thereby reducing the dispersion of the spray. This high number concentration also promotes coalescence. As the spray approaches the wall, secondary breakup of the coalesced globules are observed (globule size is proportional to symbol size).

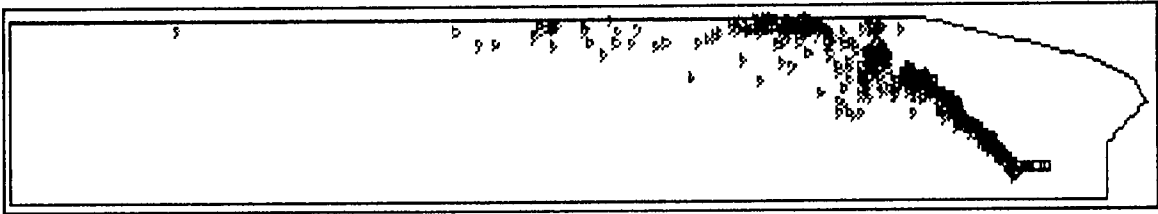


Figure 37. Computed spray structure for N₂H₄/LOX spray combustion in a VTE.

The gas velocity field is shown in Figure 38. An interesting feature of the velocity field is the appearance of an outer recirculation zone and a small inner shear layer. This is in contrast to the double recirculation zone pattern usually observed. It can be seen that along the chamber axis near the point of impingement there is a relatively high velocity region created by gases flowing out of the recirculation zone. Note that the details of the pintle geometry are not resolved thereby preventing any definite conclusions to be drawn about the local gas flow near the injection port.

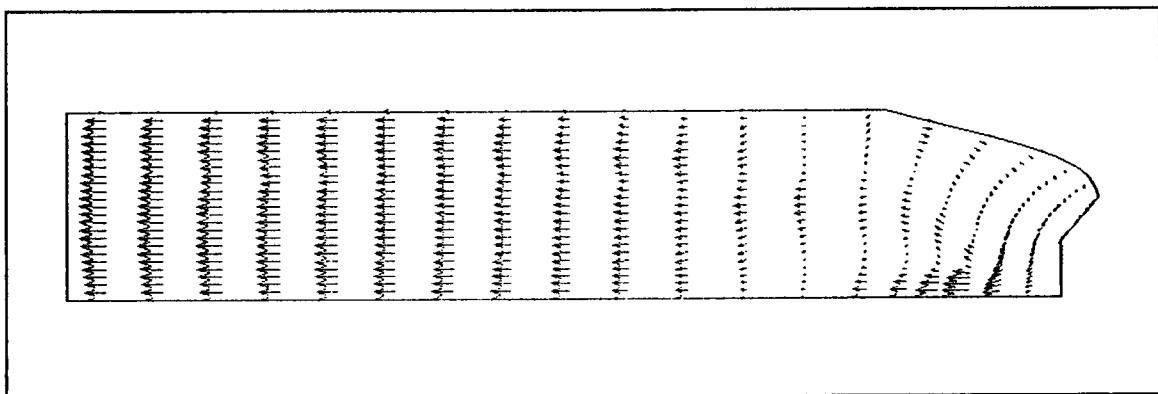


Figure 38. Gas velocity field for N₂H₄/LOX spray combustion in a VTE.

The gas temperature field is shown in figure 39. Combustion is observed

to occur in the outer portion of the chamber. The contoured portion of the injection region acts as a flame holder with hot combustion products being entrained by the recirculation vortex. There is a relatively cool (i.e., 500 K) region near the impingement point. The hot gases being ejected out of the recirculation zone do not penetrate this cool region but rather, detour around it. Hence, the creation of the shear layer with high velocity hot gas at the axis and cool gas flowing on top. This cool region is sustained by vaporization of large drops resulting from coalescence and also the high globule number density that is injected.

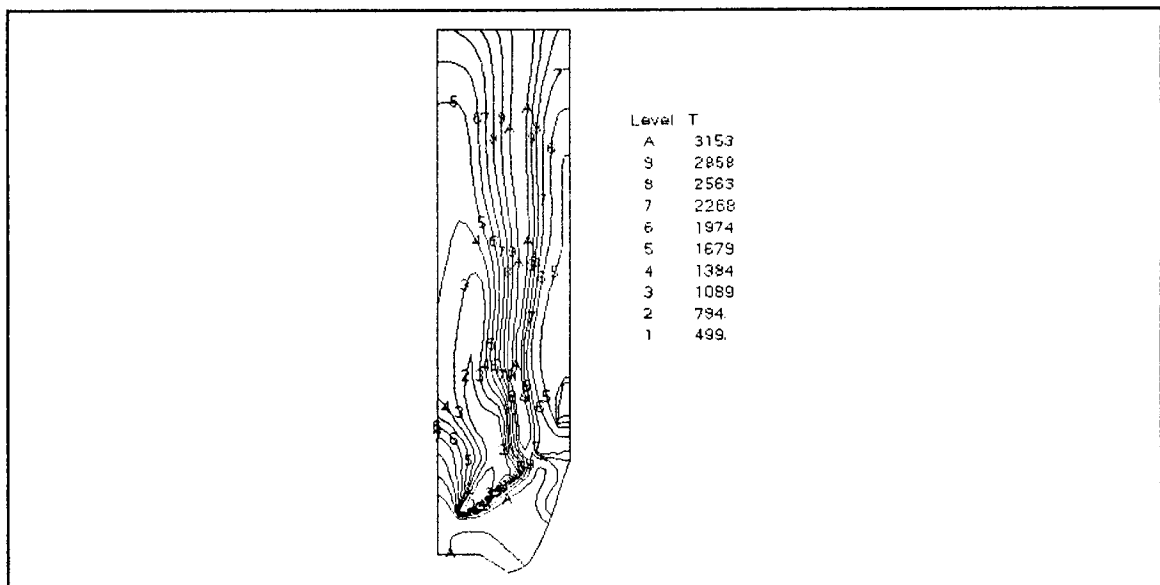


Figure 39. Gas temperature field for N₂H₄/LOX spray combustion in a VTE.

Species mass fraction contours are presented in Figures 41 and 42. Most of the N₂H₄ fuel is completely consumed. A significant concentration of O₂ vapor is established near the combustor axis. Mass fraction contours for the primary

combustion products (N_2 , H_2O) confirm this outer zone combustion characteristic of this combustor configuration.

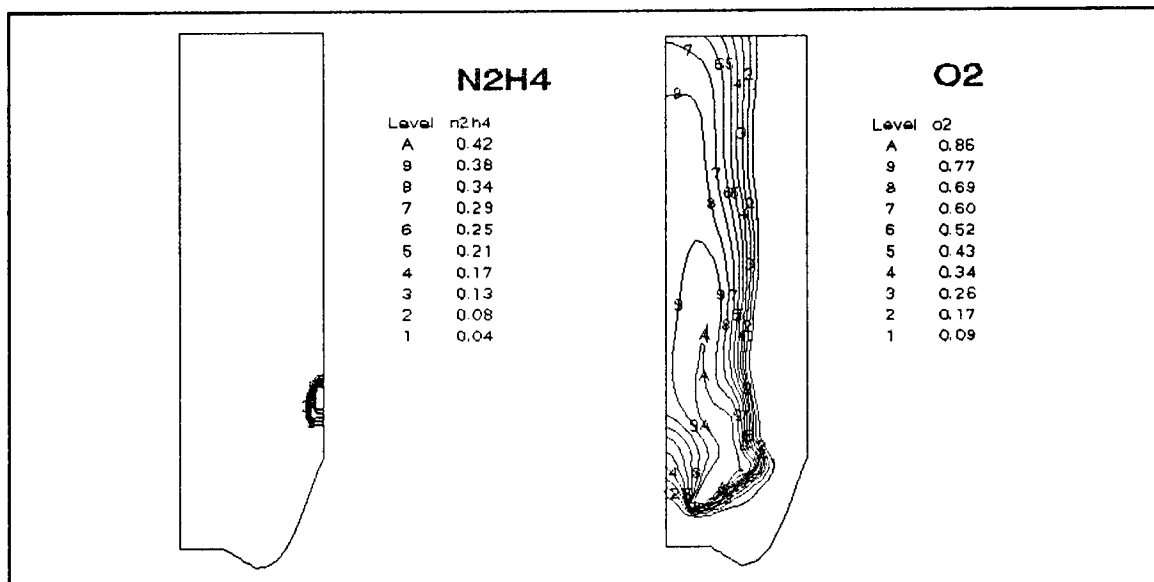


Figure 40. N_2H_4 and O_2 species mass fraction contours for VTE spray combustion.

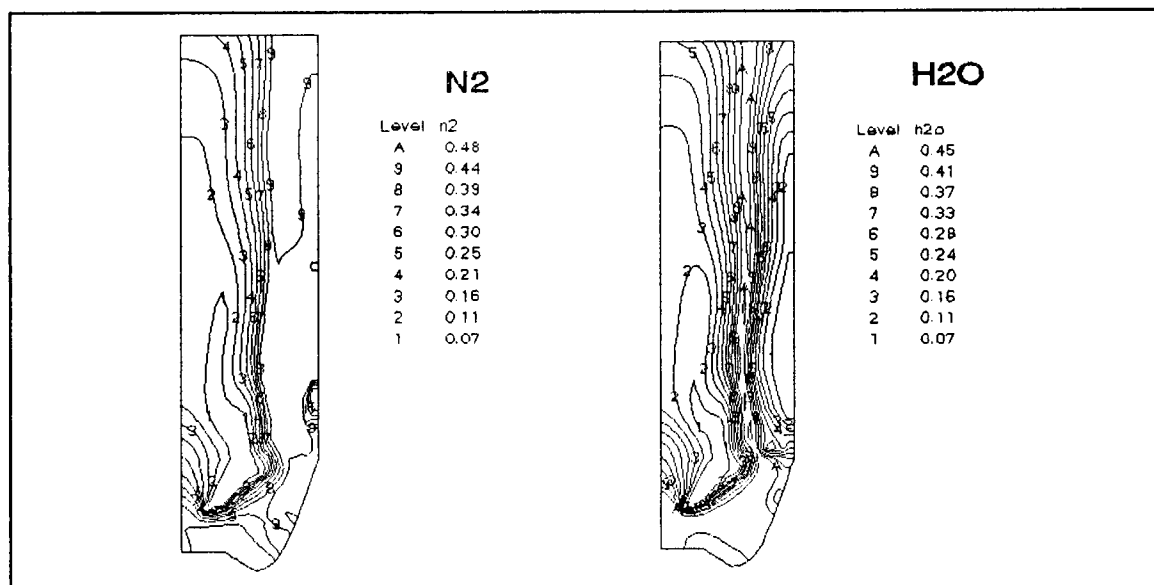


Figure 41. Primary combustion products for VTE spray combustion.

Performance improvements may be obtained for this configuration by promoting more oxidizer and fuel mixing near the chamber axis. The thin spray structure that is observed indicates a need for methods that will create a more dispersed spray pattern thereby directing some of the fuel towards the chamber axis. A study on the effect of varying spray cone angle was performed to see what benefits can be reaped. For this study, a spray axis of 50 degrees was assumed and fuel and oxidizer sprays with a Rosin-Rammler size distribution were injected. The stream impingement and atomization/breakup models were turned off. An SMR of 20 microns was assumed based upon the computed value from the baseline case employing the atomization/breakup model. Cone angles of 20, 60, and 100 degrees about the spray axis were specified.

Figure 42 shows the effect of varying cone angle on the velocity field. reducing the cone angle produces a less uniform velocity field and moves the core of the outer recirculation zone closer to the impingement region. This results in high velocities in the outer portion of the chamber and low velocities near the axis. The inner shear layer region is not significantly affected for the 60 and 20 degree cases. A developing inner recirculation zone is observed for the 100 degree case. The gas temperature field is shown in Figure 43 for the three cases. It can be observed that increasing the cone angle reduces the extent of the cool zone near the chamber axis. A more uniform temperature profile is produced at the combustor exit as the cone angle is increased.

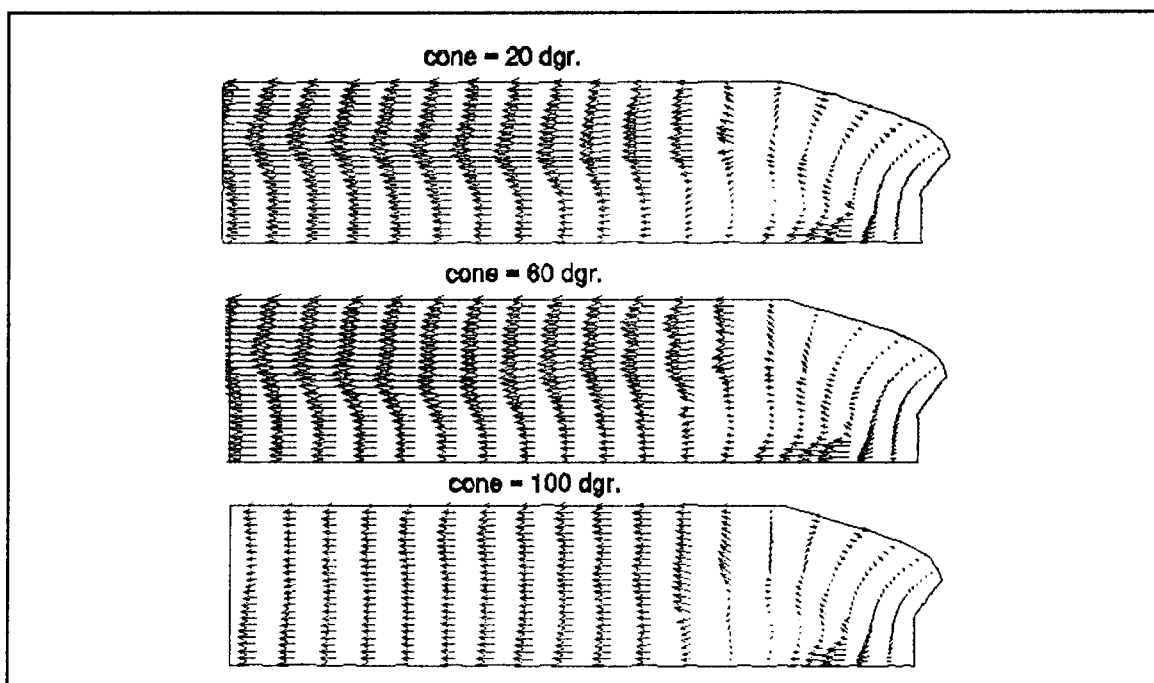


Figure 42. Effect of varying spray cone angle on the velocity field for VTE spray combustion.

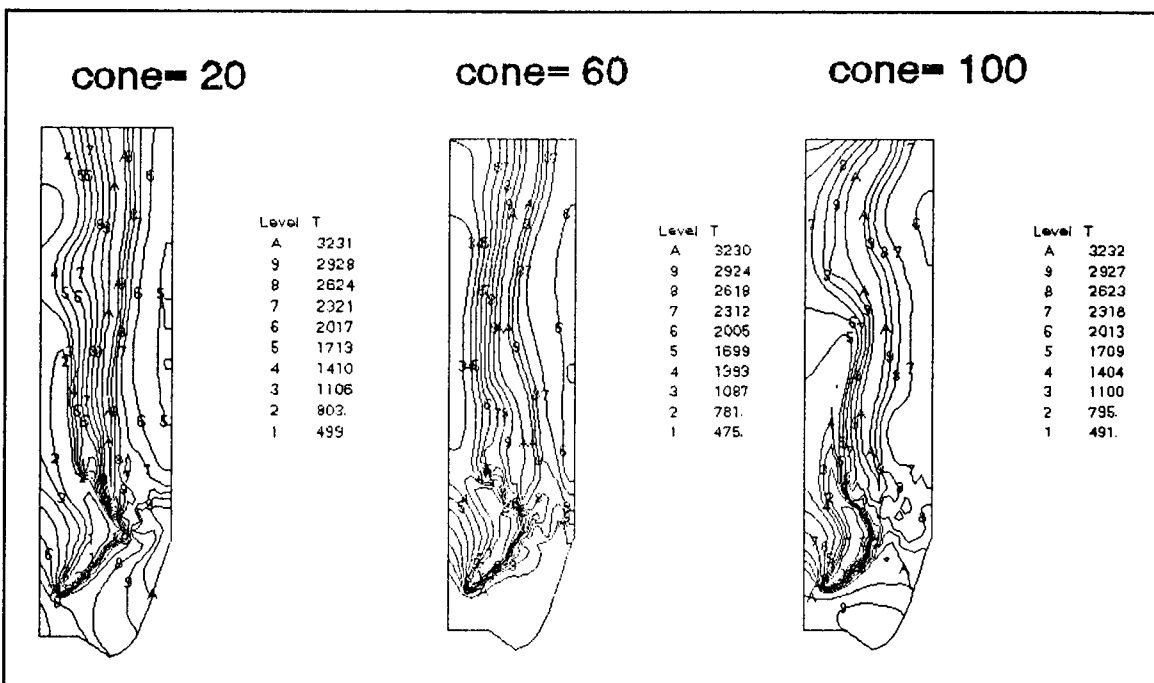


Figure 43. Effect of varying spray cone angle on the temperature field for VTE spray combustion.

Thus, it is shown that making the spray more dispersed through an increase in the cone angle produces more uniform properties at the combustor exit. The mechanisms for producing a more dispersed spray with a coaxial pintle injector are beyond the scope of this work. Not much is known about the characteristics of this type of injector. A fully three-dimensional treatment may be required to better analyze the spray patterns from this type of impinging stream injector. The effect of tilting the spray more towards the chamber axis was not investigated in detail but intuitively, this route would not seem to be beneficial in regards to gas/wall compatibility.

6 CONCLUDING REMARKS

A local diagnostic tool has been developed for analyzing the bipropellant spray combustion and flow structure within small rocket combustors. Applications were presented that demonstrated the capabilities of the current approach. Although there has not been any complete validation of this model, the following remarks can be stated:

- (1) Gross spray characteristics such as global structure (i.e., shape, cone angle) and size distribution seem to be qualitatively well simulated by this model for single element impinging doublet injectors. Reasonable quantitative agreements with established correlations have also been obtained for the atomized spray sizes that are produced.
- (2) Insights into the development of a bipropellant spray within a reactive gas have been given. The computed results seem rationally plausible and are in qualitative accord with similar work that have been performed.
- (3) For small rocket engine development, relative effects of hardware modifications can be quickly investigated with the current approach. A demonstration of such an application was given.

Benchmark experimental validation of this model is essential for establishing its usefulness. It is hoped that the needed test data will be forthcoming.

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APPENDIX

APPENDIX

Derivation of Turbulence KE Equation

The derivation of the averaged fluctuation KE equation (2.28) is very tedious but straightforward. A sketch of the primary steps follows.

By considering the scalar product of $\tilde{u}_j$ and the averaged momentum equation for $\tilde{u}_i$,

$$\tilde{u}_j \left\{ \frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_k}{\partial x_k} = - \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_k} [\bar{\tau}_{jk} - \bar{\rho} \widetilde{u_j'' u_k''}] + F_i^s \right\}$$

and the scalar product of $\tilde{u}_i$ and the mean momentum equation for $\tilde{u}_j$,

$$\tilde{u}_i \left\{ \frac{\partial \bar{\rho} \tilde{u}_j}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_k}{\partial x_k} = - \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_k} [\bar{\tau}_{jk} - \bar{\rho} \widetilde{u_j'' u_k''}] + F_j^s \right\}$$

and adding these two equations and rearranging, we obtain for $i=j$

$$\begin{aligned} \frac{\partial}{\partial t} \left(\bar{\rho} \frac{\tilde{u}_i \tilde{u}_i}{2} \right) + \frac{\partial}{\partial x_k} \left(\bar{\rho} \frac{\tilde{u}_i \tilde{u}_i}{2} \tilde{u}_k \right) = & - \tilde{u}_i \frac{\partial \bar{p}}{\partial x_i} + \\ & \tilde{u}_i \frac{\partial}{\partial x_k} [\bar{\tau}_{ik} - \bar{\rho} \widetilde{u_i'' u_k''}] + \tilde{u}_i F_i^s - \frac{\tilde{u}_i \tilde{u}_i}{2} \dot{\rho}^s. \end{aligned} \quad (\text{A.1})$$

The last two terms in equation (A.1) are due to the liquid/gas interfacial interactions. An equation for the instantaneous gas phase kinetic energy may be obtained in a manner analogous to what is done for the averaged KE equation

(eq. A.1). Performing the steps result in

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u_i u_j) + \frac{\partial}{\partial x_k}(\rho u_i u_j u_k) = & -\frac{\partial \rho u_j}{\partial x_i} + \rho \frac{\partial u_j}{\partial x_i} - \frac{\partial \rho u_i}{\partial x_j} + \\ & \rho \frac{\partial u_i}{\partial x_j} + \frac{\partial \tau_{jk} u_j}{\partial x_k} - \tau_{jk} \frac{\partial u_j}{\partial x_i} + \frac{\partial \tau_{jk} u_i}{\partial x_k} - \tau_{jk} \frac{\partial u_i}{\partial x_k} . \end{aligned} \quad (\text{A.2})$$

Letting $j=i$ in equation (A.2), taking the non-intrinsic average and subtracting from equation (A.1) lead to equation (2.28).

VITA

Louis M. Larosiliere was born in Port-au-Prince, Haiti on July 16, 1960. His secondary education was formed at parochial schools in Boston, Massachusetts and he graduated from Boston College High School. He received a Bachelor of Science degree in Aerospace Engineering from Boston University. Soon after, he was awarded a Master of Science Degree from the University of Tennessee at Knoxville. Mr. Larosiliere was employed by Sverdrup Technology inc. at AEDC as a propulsion analysis engineer. After leaving Sverdrup, he received a Post-Graduate Diploma in fluid dynamics from the von Karman Institute in Belgium. He then worked in the turbomachinery aerodynamics field at the General Electric Co. and also at Williams International. He continued his graduate study at the University of Tennessee Space Institute and was awarded a doctor of philosophy in Aerospace Engineering in 1991.