SPRAY COMBUSTION MODELING WITH VOF AND FINITE-RATE CHEMISTRY

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ABSTRACT

A spray atomization and combustion model is developed based on the volume-of-fluid (VOF) transport equation with finite-rate chemistry model. The gas-liquid interface mass, momentum and energy conservation laws are modeled by continuum surface force mechanisms. A new solution method is developed such that the present VOF model can be applied for all-speed range flows. The objectives of the present study are: (a) to develop and verify the fractional volume-of-fluid (VOF) cell partitioning approach into a predictor-corrector algorithm to deal with multiphase (gas-liquid) free surface flow problems; (b) to implement the developed unified algorithm in a general purpose computational fluid dynamics (CFD) code, Finite Difference Navier-Stokes (FDNS), with droplet dynamics and finite-rate chemistry models; and (c) to demonstrate the effectiveness of the present approach by simulating benchmark problems of jet breakup/spray atomization and combustion. Multiphase fluid flows involving free surface fluids can be found in many space transportation and propulsion systems such as injector atomization in Space Shuttle Main Engine (SSME) combustors, cavitation in liquid rocket pump operations, handling of cryogenic liquids in a micro-gravity environment and the operation of cryogenic propellants on board spacecraft. Modeling these types of flows poses a significant challenge because a required boundary must be applied to a transient, irregular surface that is discontinuous, and the flow regimes considered can range from incompressible to high-speed compressible flows. The flow-process modeling is further complicated by surface tension, interfacial heat and mass transfer, spray formation and turbulence, and their interactions.

The major contribution of the present method is to combine the novel feature of the Volume of Fluid (VOF) method and the Eulerian/Lagrangian method into a unified algorithm for efficient non-iterative, time-accurate calculations of multiphase free surface flows valid at all speeds. The proposed method reformulated the VOF equation to strongly couple two distinct phases (liquid and gas), and tracks droplets on a Lagrangian frame when spray model is required, using a unified predictor-corrector technique to account for the non-linear linkages through the convective contributions of VOF. The discontinuities within the sharp interface will be modeled as a volume force to avoid stiffness. Formations of droplets, tracking of droplet dynamics and modeling of the droplet breakup/evaporation, are handled through the same unified predictor-corrector procedure. Thus the new algorithm is non-iterative and is flexible for general geometries with arbitrarily complex topology in free surfaces. The FDNS finite-difference Navier-Stokes code is employed as the baseline of the current development.

Benchmark test cases of shear coaxial LOX/H2 liquid jet with atomization/combustion and impinging jet test cases are investigated in the present work. Preliminary data comparisons show good qualitative agreement between data and the present analysis. It is indicative from these results that the present method has great potential to become a general engineering design analysis and diagnostics tool for problems involving spray combustion.

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Overview

- INTRODUCTION
- THEORETICAL APPROACH
- NUMERICAL METHOD
- SHEAR COAXIAL INJECTOR TEST CASES
- IMPINGING INJECTOR TEST CASES
- FUTURE WORK

INTRODUCTION

- FLUID DYNAMICS PROBLEMS WITH MULTI-PHASE INTERFACE ARE IMPORTANT IN MANY ENGINEERING DESIGN APPLICATIONS SUCH AS INJECTOR SPRAY BREAKUP/ ATOMIZATION, SPRAY COATING, CRYOGENIC FLUID MANAGEMENT, MATERIAL PROCESSING, CRYSTAL GROWTH, CHEMICAL VAPOR DEPOSITION AND CAVITATION/ CONDENSATION, ETC.

- MAJOR DIFFICULTIES IN NUMERICAL MODELING INVOLVE LARGE DENSITY JUMP ACROSS INTERFACE, CALCULATION OF SURFACE TENSION FORCE IN 3-D SPACE AND IMPORTANT EFFECTS OF MATERIAL PROPERTY VARIATIONS.

- VOLUME OF FLUID (VOF) METHOD USES FLUID VOLUME TRANSPORT EQUATION ON EULERIAN FRAMEWORK -- RESOLUTION OF THE INTERFACE IS AN IMPORTANT ISSUE. VOF METHOD IS GENERAL AND CAN BE APPLIED TO COMPLEX INTERFACE GEOMETRY PROBLEMS.

- WITH VOF INTERFACE MODELING, LAGRANGIAN PARTICLE TRACKING METHOD AND FINITE-RATE CHEMISTRY MODELS, SPRAY ATOMIZATION/ COMBUSTION PROCESSES CAN BE SIMULATED. A SPRAY COMBUSTION MODEL DEVELOPED BASED ON THESE FEATURES CAN BE VERY USEFUL IN THE ANALYSIS OF INJECTOR/COMBUSTION CHAMBER DESIGN AND DIAGNOSIS ISSUES.

THEORETICAL APPROACH

- CONSERVATION EQUATIONS FOR THE LIQUID, WHICH IS INCOMPRESSIBLE, AND FOR THE GAS FLOW WHICH IS COMPRESSIBLE.
- VOLUME OF FLUID TRANSPORT EQUATION USED TO PREDICT THE INTERFACE DYNAMICS.
- CONTINUUM SURFACE FORCE MODEL IS EMPLOYED TO MODEL THE SURFACE TENSION FORCE.
- LAGRANGIAN PARTICLE TRACKING METHOD FOR TREATING THE DYNAMICS AND HEAT/MASS TRANSFER OF PARTICLE PARCELS IN STATISTICAL SENSE.
- MULTI-COMPONENT FINITE-RATE CHEMISTRY MODEL BASED ON POINT IMPLICIT AND PENALTY FUNCTION APPROACH.

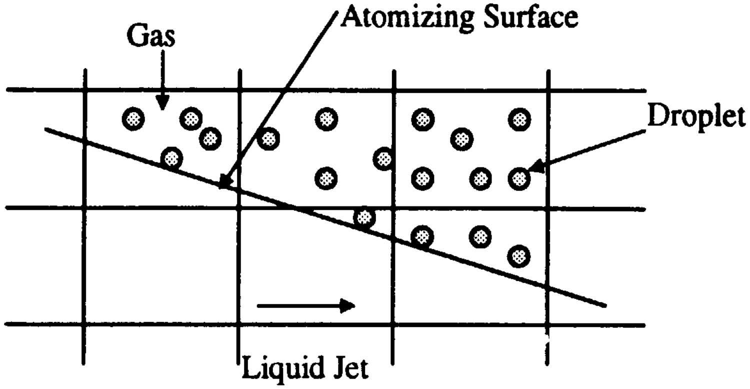
Transport Equations

For flow variables:

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \left(u - u_g\right)_i \phi}{\partial x_i} = D_\phi + S_\phi$$

and for VOF equation:

$$\frac{\partial \alpha}{\partial t} + \left(u - u_g\right)_i \frac{\partial \alpha}{\partial x_i} = S_\alpha$$



Implementation of atomization and spray model

where $\alpha = 1$ stands for liquid and $\alpha = 0$ is for gas. The interface is located at $1 > \alpha > 0$.

For a given solution of α field, the governing equations can be recast as:

$$\frac{\partial \rho_m \phi}{\partial t} + \frac{\partial \rho_m \left(u - u_g\right)_i \phi}{\partial x_i} = D_\phi + S_\phi, \quad \alpha < 0.05 \text{ -------- for compressible gas}$$

$$\rho_m \frac{\partial \phi}{\partial t} + \rho_m \left(u - u_g\right)_i \frac{\partial \phi}{\partial x_i} = D_\phi + S_\phi, \quad \alpha \geq 0.05 \text{ -------- for interface and liquid}$$

where

$$\rho_m = (1-\alpha)\rho_g - \alpha\rho_l$$

where ρ_g and ρ_l denote gas and liquid density respectively. u_g represents the grid speed components used to simulate moving domain effects.

Continuum Surface Force Model

Surface Tension Forces:

$$F_x = -\sigma\left(\nabla \hat{n}\right)\alpha_x$$

$$F_y = -\sigma\left(\nabla \hat{n}\right)\alpha_y + \left(\frac{|\alpha_y|}{y}\right)_{for\ 2D\ axisymetric\ only}$$

$$F_z = -\sigma\left(\nabla \hat{n}\right)\alpha_z\ , \quad --- for\ 3D\ case\ only$$

where

σ = surface tension constant

$\nabla \hat{n} = \hat{\alpha}_{xx} + \hat{\alpha}_{yy} + \hat{\alpha}_{zz}$

Spray Atomization Model

- Reitz & Diwakar Wave Instability Atomization Model
- CICM (Coaxial Injector Combustion Model) Atomization Model (Liang & Jensen)
- Mass Stripping Rates Applied to the VOF Equation Along the Interface for the Liquid Core Prediction

Pressure Sensitivity Analysis

- Case D of Penn State Experiment:

Pc = 443 psia;
injector diameter = 3.43 mm;
gas velocity = 840 m/s;
liquid velocity = 18 m/s;
gas temperature = 300 K;
liquid temperature = 106 K; and
gas density = 2.48 kg/m**3.

Table 1. Comparisons of Spray Atomization Models

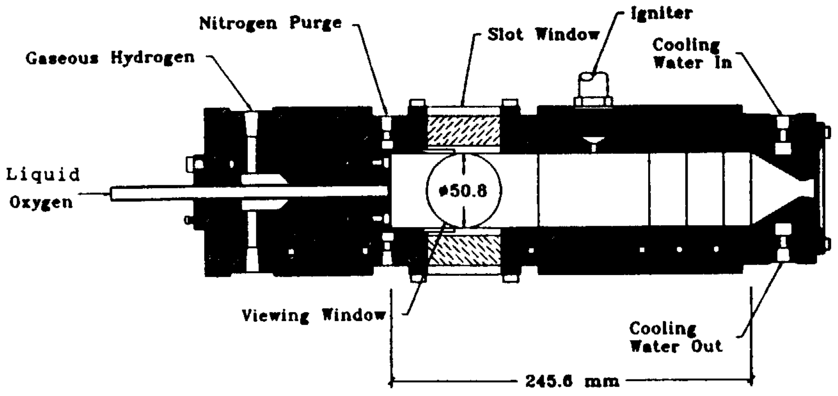
	Mean Droplet Size (μm)			
P (ATM)	10	20	40	300
Reitz Model	0.122	0.0636	0.0334	0.0054
CICM Model	3.22	2.03	1.28	0.334

NUMERICAL METHOD

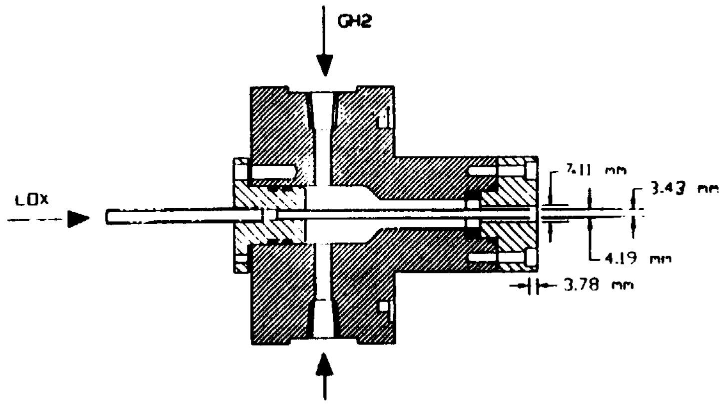
- PREDICTOR-CORRECTOR TIME MARCHING ALGORITHM BASED ON FDNS
  - -- UNIFIED SOLUTION FOR INCOMPRESSIBLE LIQUID AND COMPRESSIBLE GAS
- SECOND-ORDER ARTIFICIAL DISSIPATION SCHEMES OR THIRD-ORDER UPWIND TVD SCHEMES
- CENTRAL DIFFERENCING FOR DIFFUSION, SOURCE AND SURFACE TENSION FORCE TERMS
- TURBULENCE-PARTICLE INTERACTION BASED ON THE TKE SOLUTION AND A GAUSSIAN FILTERED RANDOM NUMBER GENERATOR
- HIGH-ORDER TVD SCHEME FOR VOF TRANSPORT EQUATION FOR GOOD INTERFACE RESOLUTION

COAXIAL INJECTOR TEST CASES

- COAXIAL LIQUID JET ATOMIZATION
  - - KEROSENE/O2 INJECTOR ELEMENT AT 1 ATM
  - - STEADY-STATE AND TRANSIENT APPROACH
  - - WAVE INSTABILITY ATOMIZATION MODEL (Reitz & Diwakar)
- UNI-ELEMENT COMBUSTOR SIMULATION
  - - LOX/H2 COAXIAL INJECTOR (CASE D CONDITIONS OF THE PENN STATE EXPERIMENT): Real Fluid Property (NBS Table) for LOX Used.
  - - O/F RATIO OF 5.2 (Ignition initiated about the same location as the experiment)
  - - FINITE-RATE CHEMISTRY COMPUTATIONS (2-Step and 7-Step Model)

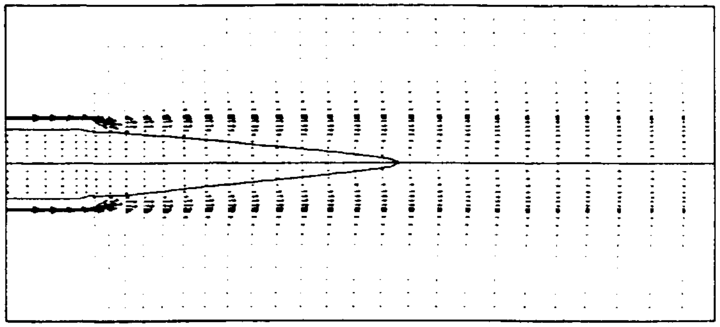


Cross-sectional view of the combustion chamber.

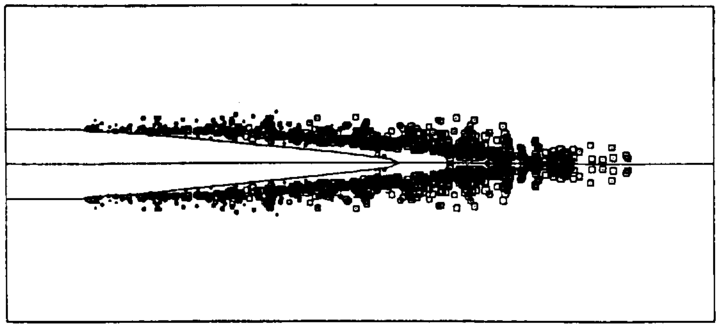


Schematic of the shear coaxial injector.

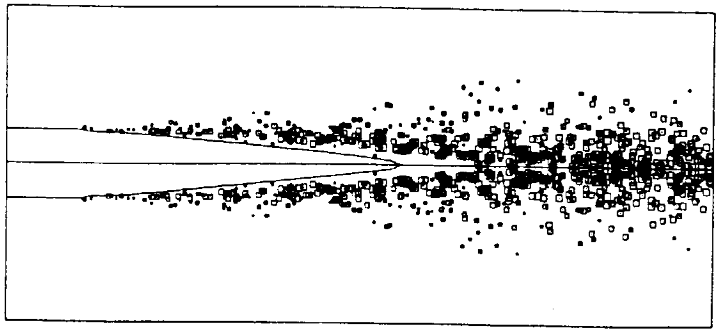
COAXIAL INJECTOR SIMULATION (1 atm, Steady-State Approach)



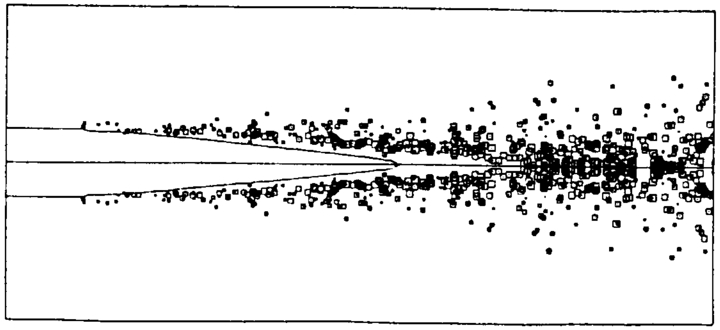
(a) Flowfield



(b) t = 0.3 ms

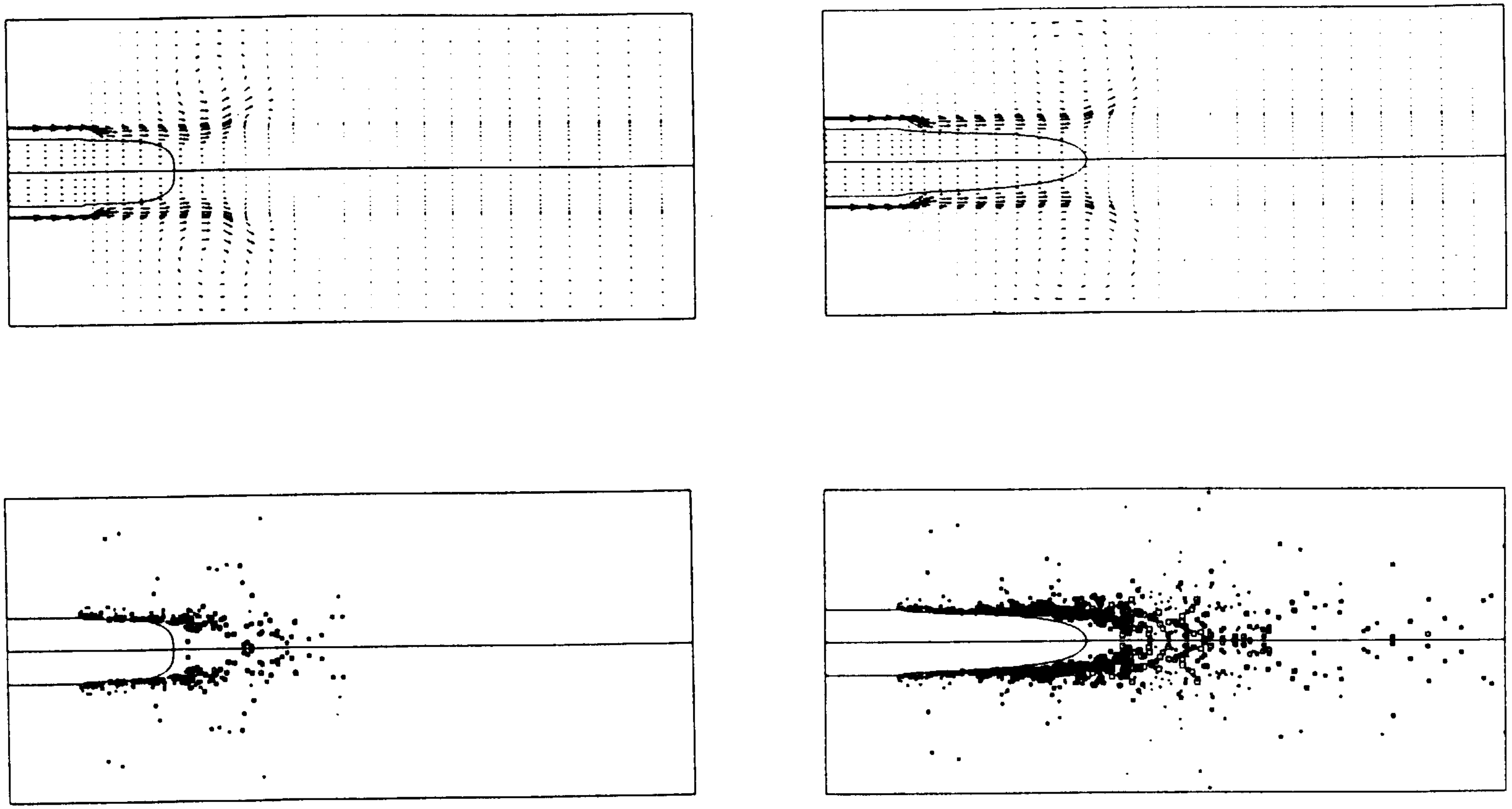


(c) t = 0.9 ms



(d) t = 1.2 ms

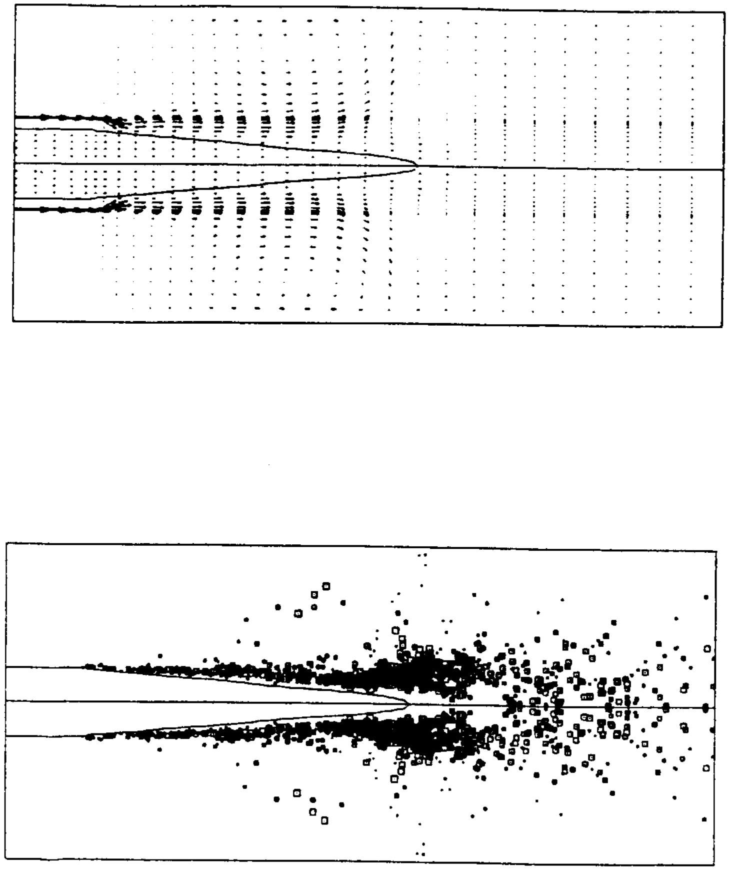
COAXIAL INJECTOR SIMULATION (1 atm, Transient Approach)



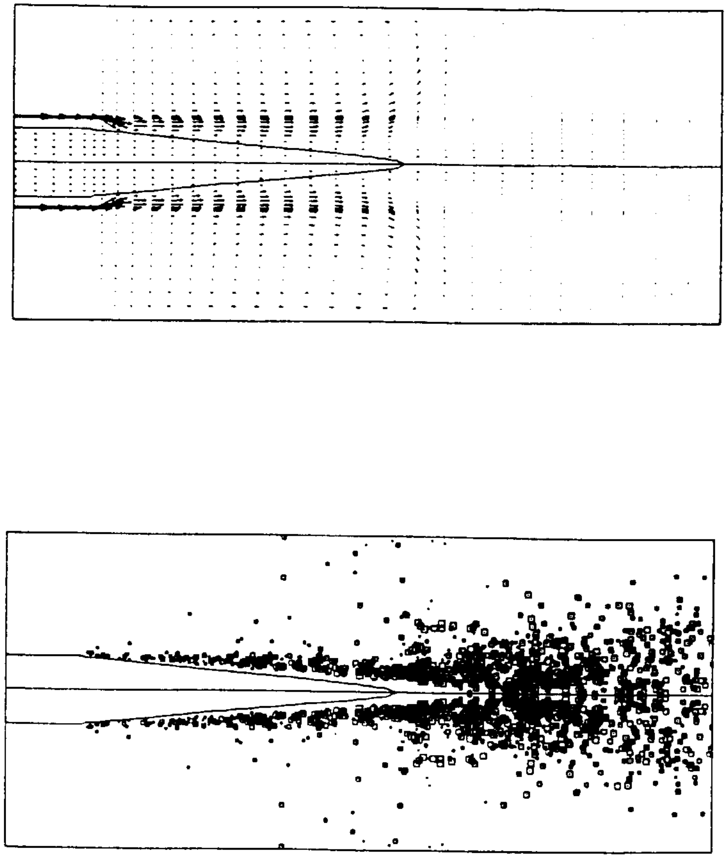
(a) t = 0.3 ms

(b) t = 0.6 ms

COAXIAL INJECTOR SIMULATION (1 atm, Transient Approach)

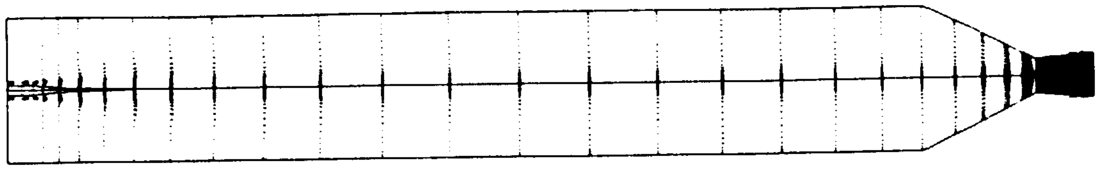


(c) t = 1.08 ms

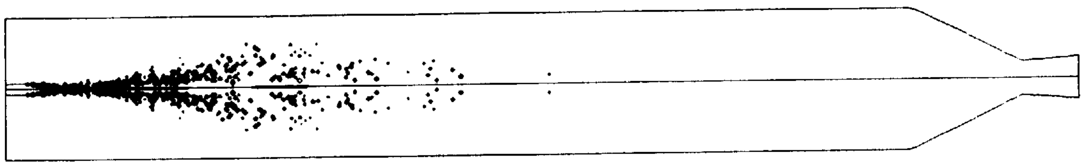


(d) t = 1.5 ms

UNI-ELEMENT COMBUSTOR SIMULATION (30 atm, 2-Step Model)

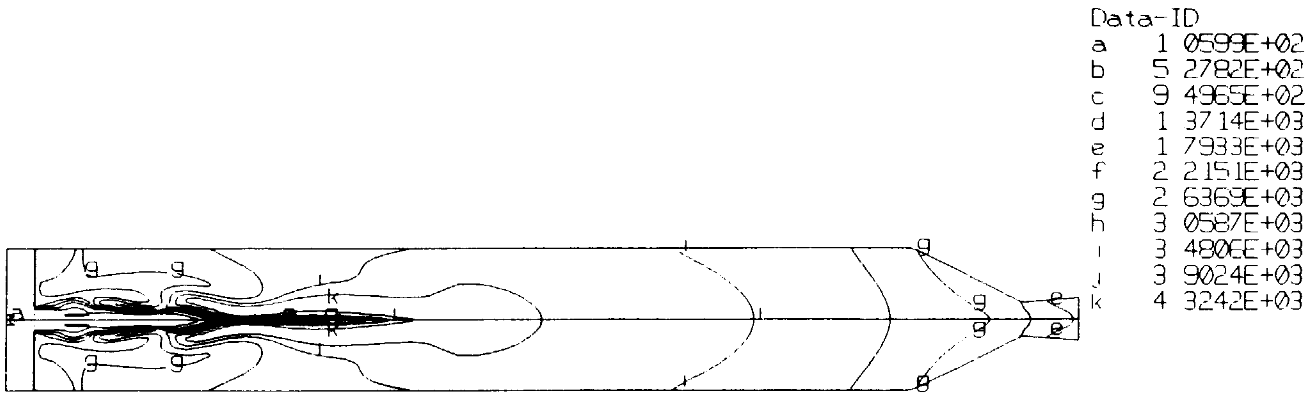


LOX Interface and Velocity Vectors

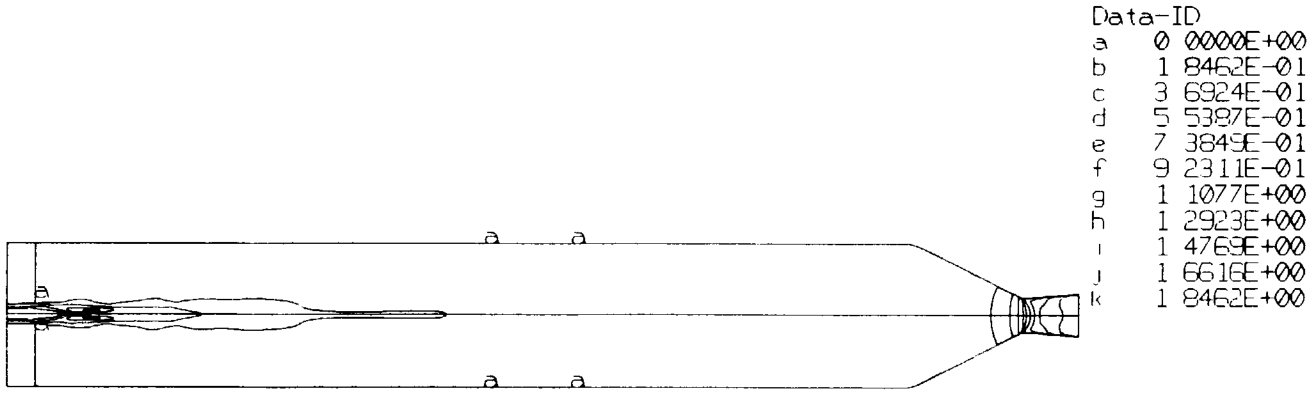


LOX Particle Plot

UNI-ELEMENT COMBUSTOR SIMULATION (30 atm, 2-Step Model)

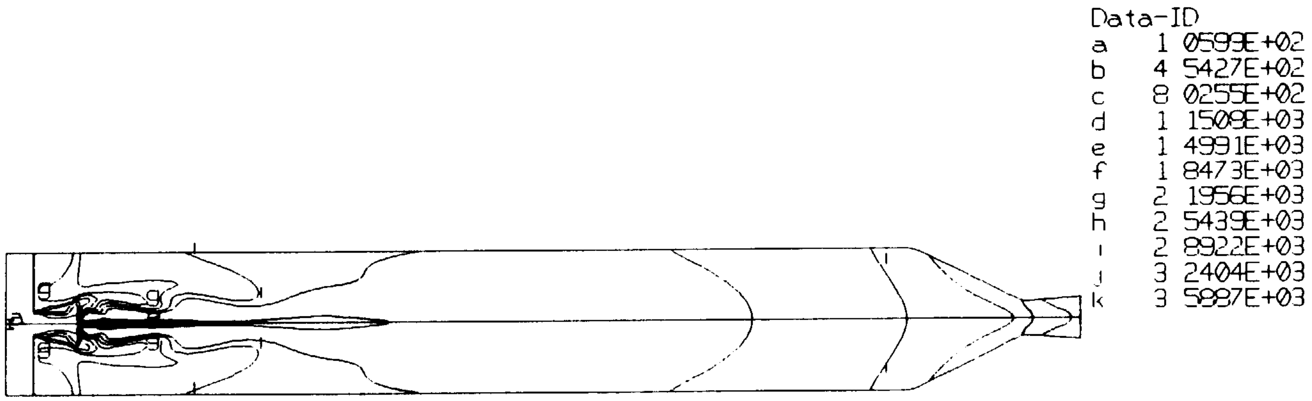


Temperature Contours (K)

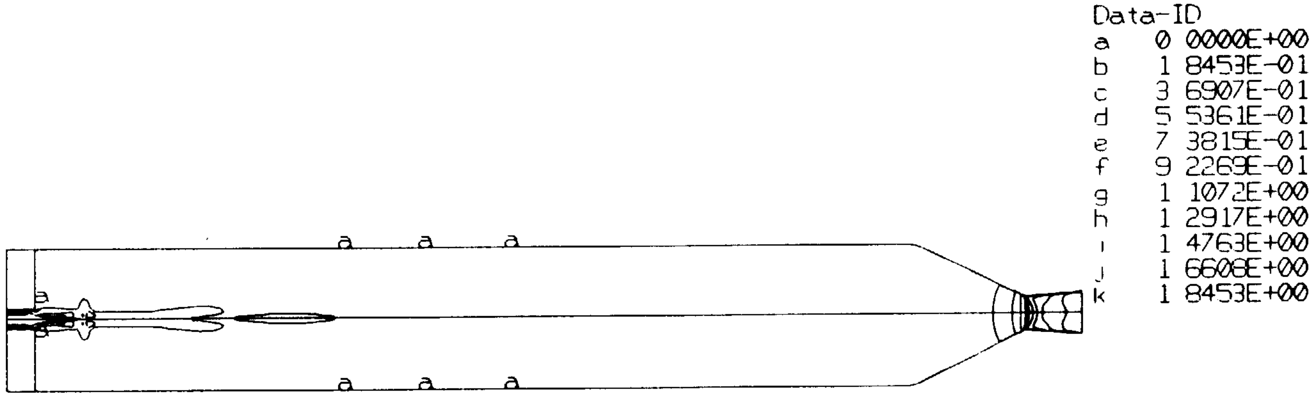


Mach Number Contours

UNI-ELEMENT COMBUSTOR SIMULATION (30 atm, 7-Step Model)



Temperature Contours (K)



Mach Number Contours

IMPINGING INJECTOR TEST CASES

- LAMINAR JET CONDITIONS FOR THEORETICAL COMPARISONS
- JET IMPINGEMENT HALF ANGLE OF 30, 60 AND 90 DEGREES
- THEORETICAL SOLUTION OF LIQUID SHEET THICKNESS DISTRIBUTION FUNCTION:

$$\frac{h*r}{R^2} = \frac{\mathrm{Sin}^2\theta}{(1-\mathrm{Cos}\phi\mathrm{Cos}\theta)^2}$$

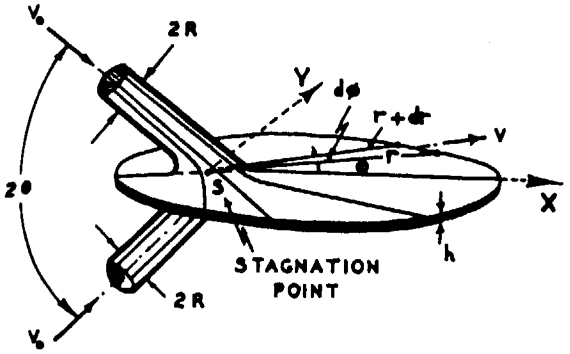
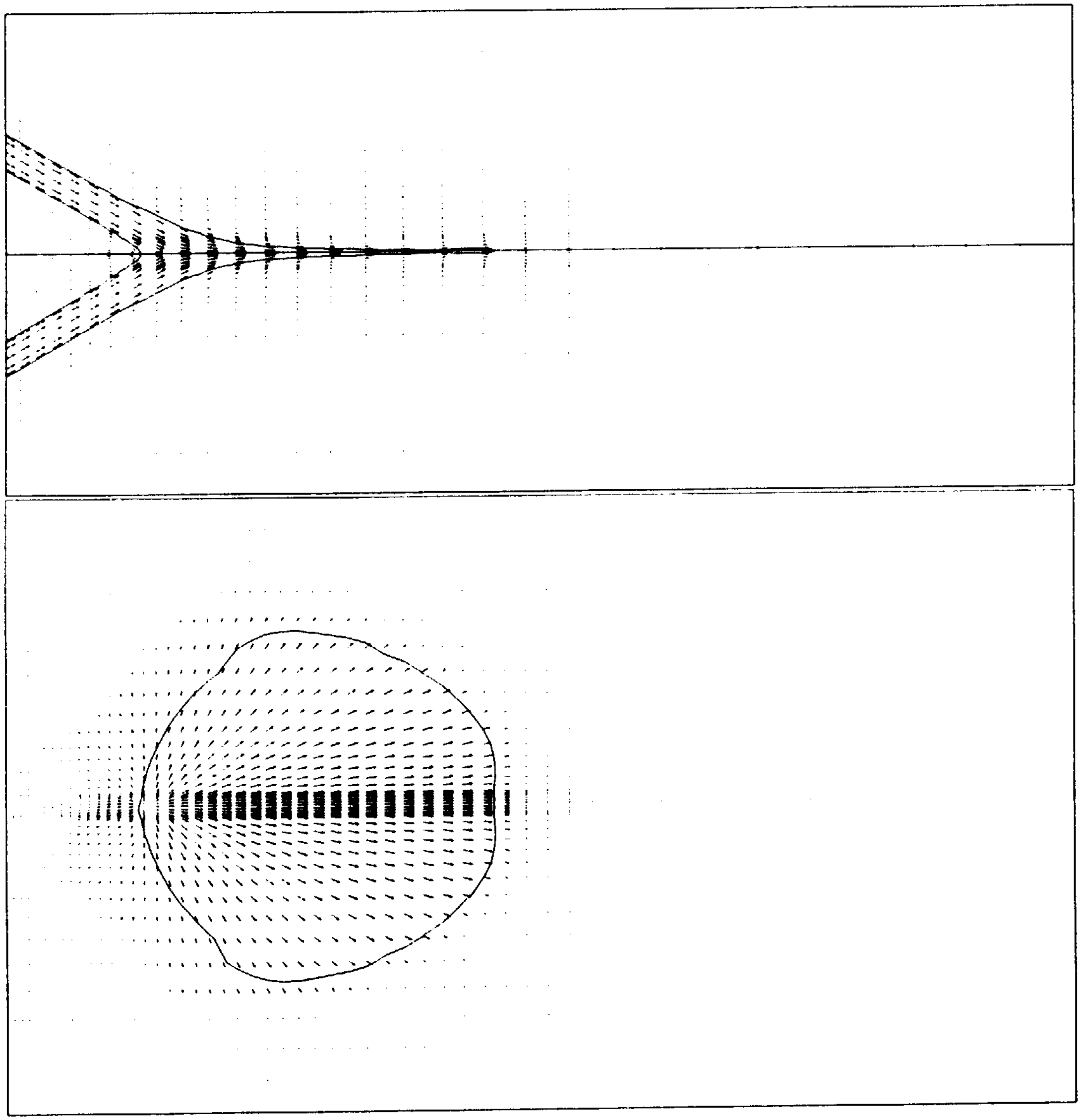
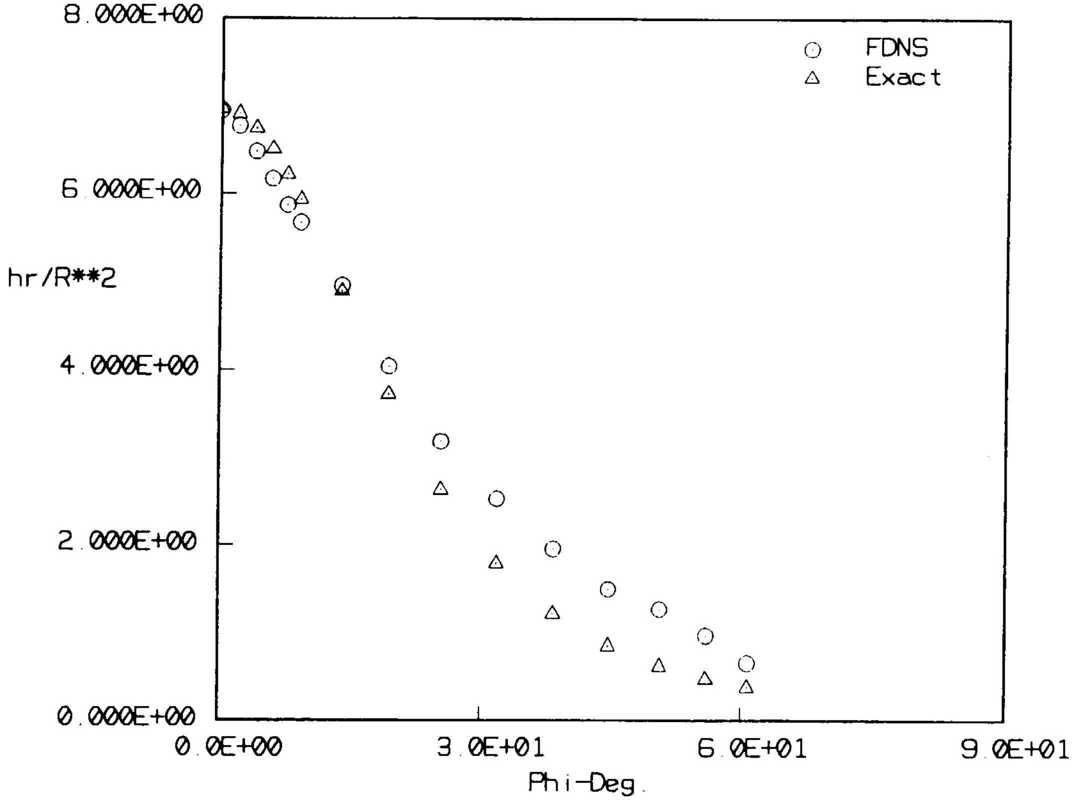


Fig. 1. Equal thickness contour of sheet formed by impinging jets.

LIQUID SHEET SURFACE ($\theta = 30°$)

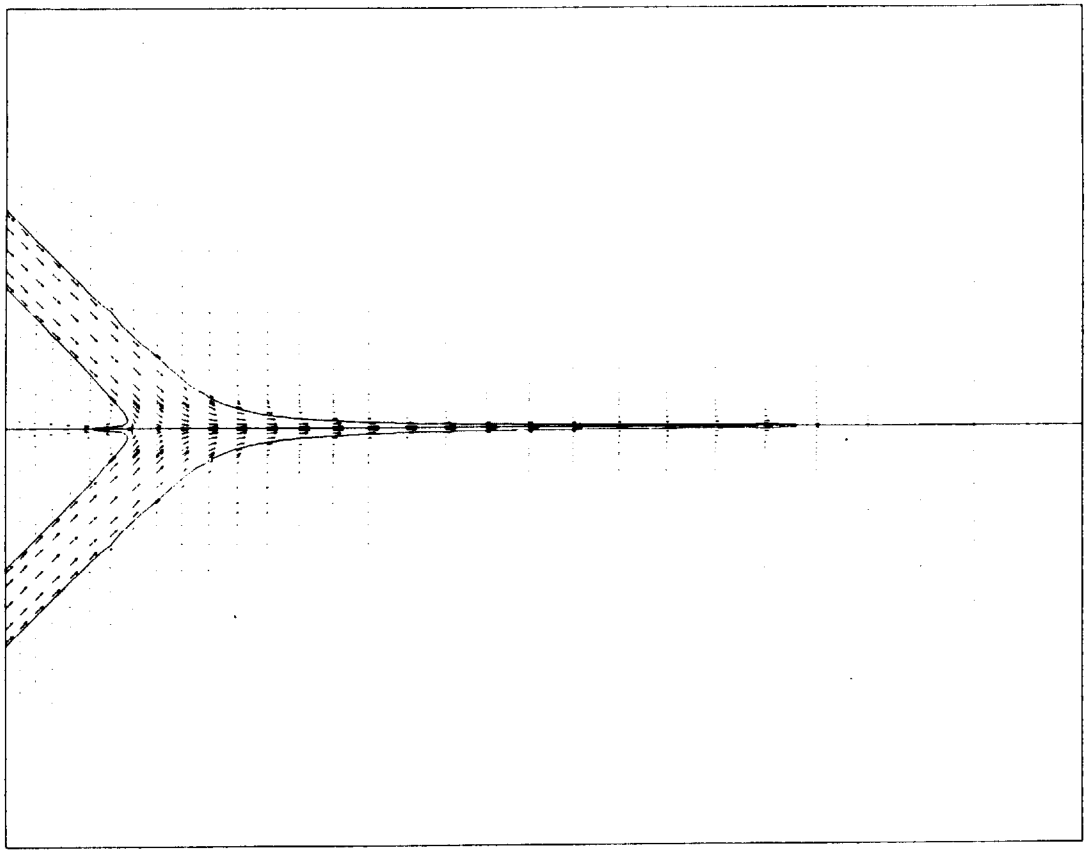


LIQUID SHEET THICKNESS COMPARISONS ($\theta = 30°$)



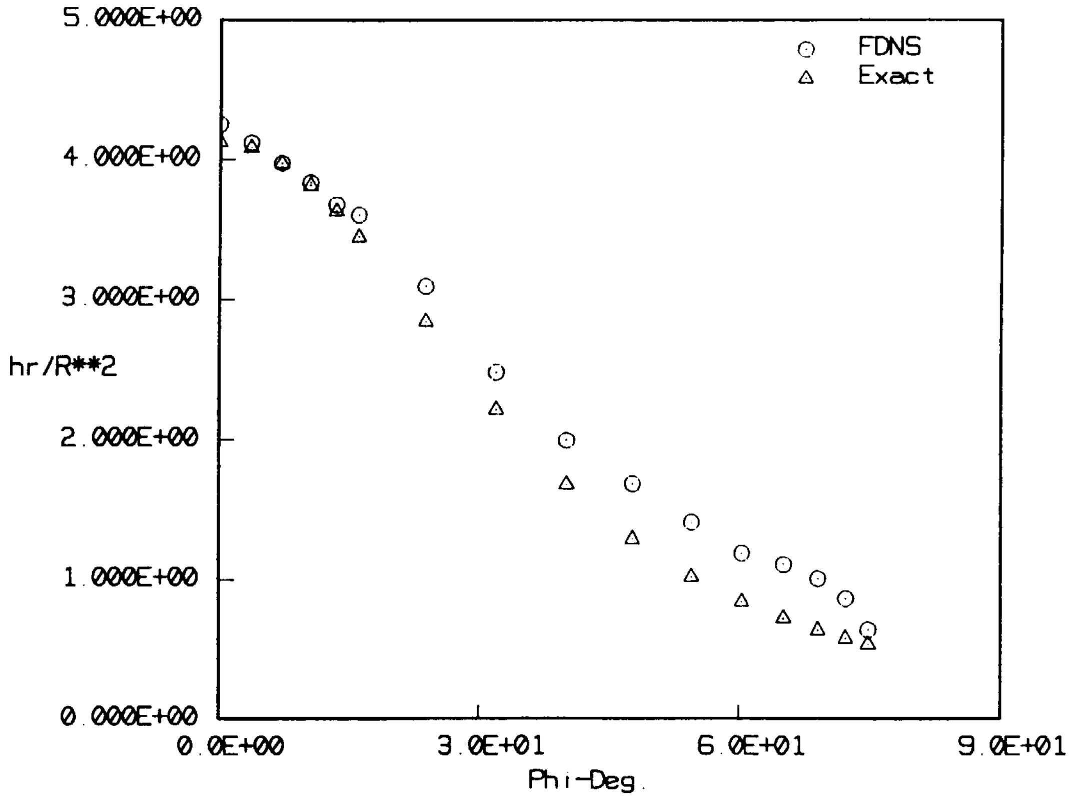
Liquid Sheet Thickness Distributions. (Theta = 30 deg.)

LIQUID SHEET SURFACE (θ = 45°)



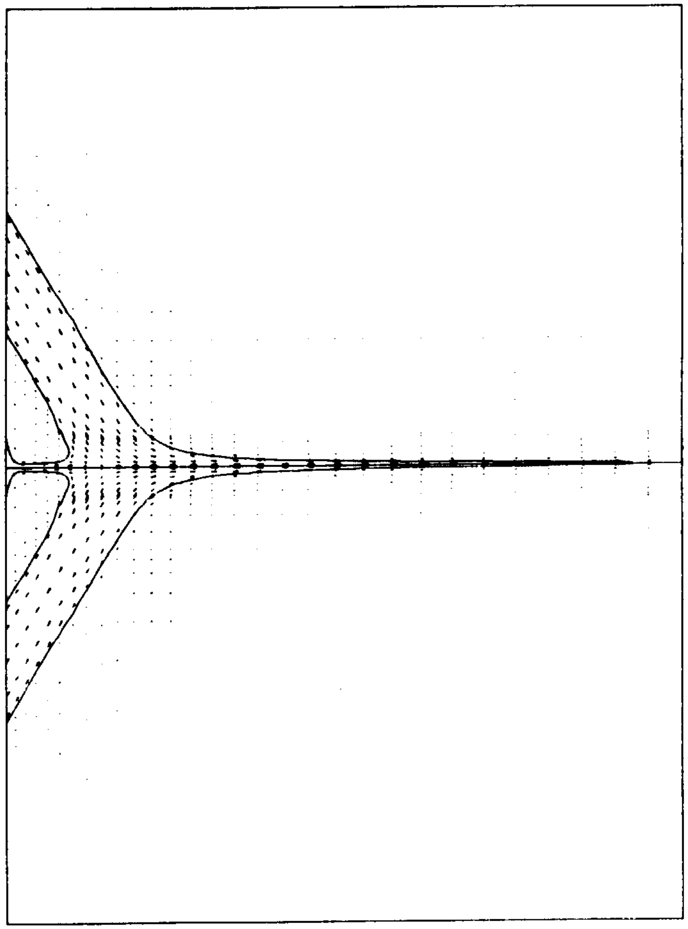
Liquid Sheet Surface (Theta = 45 deg.)

LIQUID SHEET THICKNESS COMPARISONS ($\theta = 45°$)



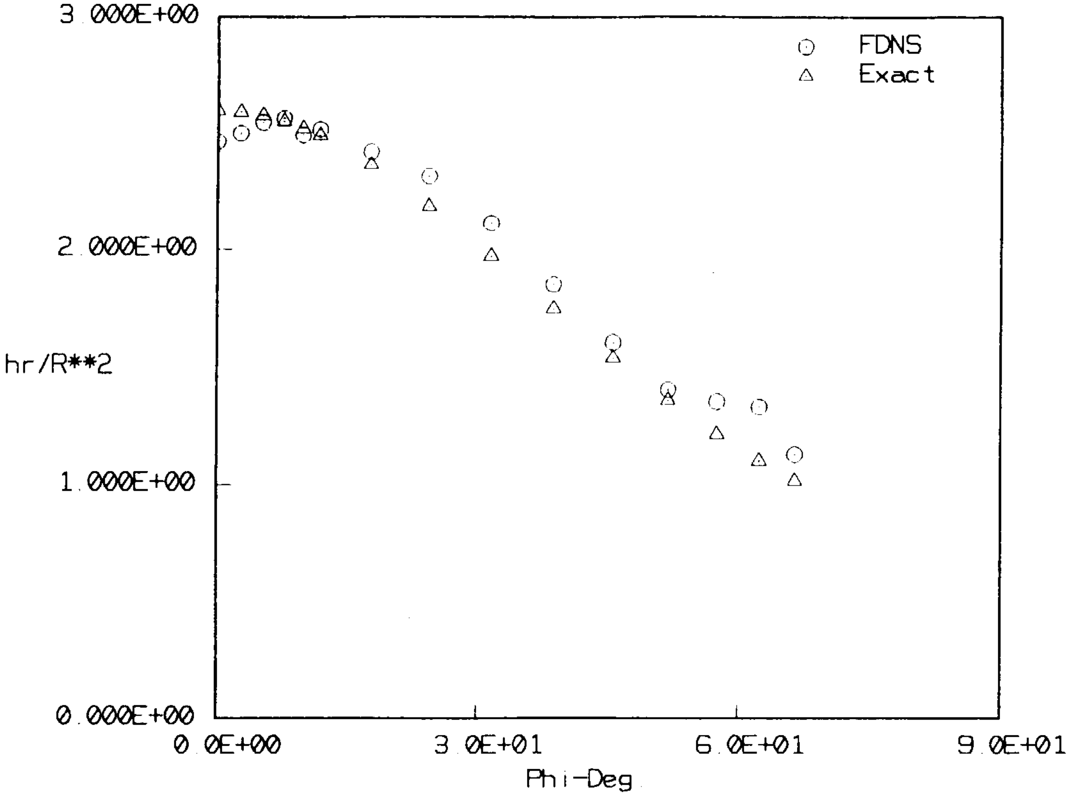
Liquid Sheet Thickness Distributions. (Theta = 45 deg.)

LIQUID SHEET SURFACE (θ = 60°)



Liquid Sheet Surface (Theta = 60 deg.)

LIQUID SHEET THICKNESS COMPARISONS (θ = 60°)



Liquid Sheet Thickness Distributions (Theta = 60 deg)

FUTURE WORK

- A GENERAL SPRAY COMBUSTION MODEL WITH VOF AND FINITE-RATE CHEMISTRY MODELS IS DEVELOPED AND BENCHMARK VALIDATION CASES ARE BEING STUDIED

- THE UNIQUENESS OF THE PRESENT METHOD IS IN ITS ALL-SPEED CAPABILITY WHICH EXPANDS THE VERSATILITY OF THE CLASSICAL VOF APPROACH

- FURTHER DEVELOPMENTAL WORK TO INCLUDE IMPINGING JETS ATOMIZATION MODEL AND VOF INTERFACE VAPORIZATION PROCESSES IN THE FDNS CODE