

**Development of an Atomization Methodology for
Spray Combustion**

S. P. Seung, C. P. Chen
Department of Chemical Engineering
University of Alabama in Huntsville
Huntsville, AL 35899

and

Y. S. Chen
Engineering Sciences Inc.

ABSTRACT

In liquid rocket propulsion, the knowledge and the understanding of liquid-gas interfacial phenomena are very important. This is of keen importance for predicting the onset of cavitation occurring in swirl injection elements used in STME, as well as atomization processes in shear-induced injector's (co-axial) and impinging injector elements. From the fact that all the physical processes including droplets size distribution, droplet dispersion, mixing and combustion are controlled by atomization processes, it is expected that the successful incorporation of the volume of fraction (VOF) will greatly enhance the analytical capability for predicting spray combustion processes in liquid-fueled engines.

In this paper, a methodology is developed to define and track interfaces between two fluids in a non-orthogonal, body-fitted grids using a single fractional volume of fluid (VOF) variable to describe the distribution of the liquid phase in a gas-liquid flow field. This method was implemented in a matured CFD code MAST (Multiphase All-Speed Transient) utilizing the general PISO-C algorithm. For the preliminary study for analyzing the spray combustion and tracking the interface between two phase, we will report the progress on simulation of the instability on the liquid column, the surface wave instability and the droplet breakup from the liquid surface.

Development of an Atomization Methodology for Spray Combustion.

**S.P. Seung, C.P. Chen
Department of Chemical Engineering
University of Alabama in Huntsville**

and

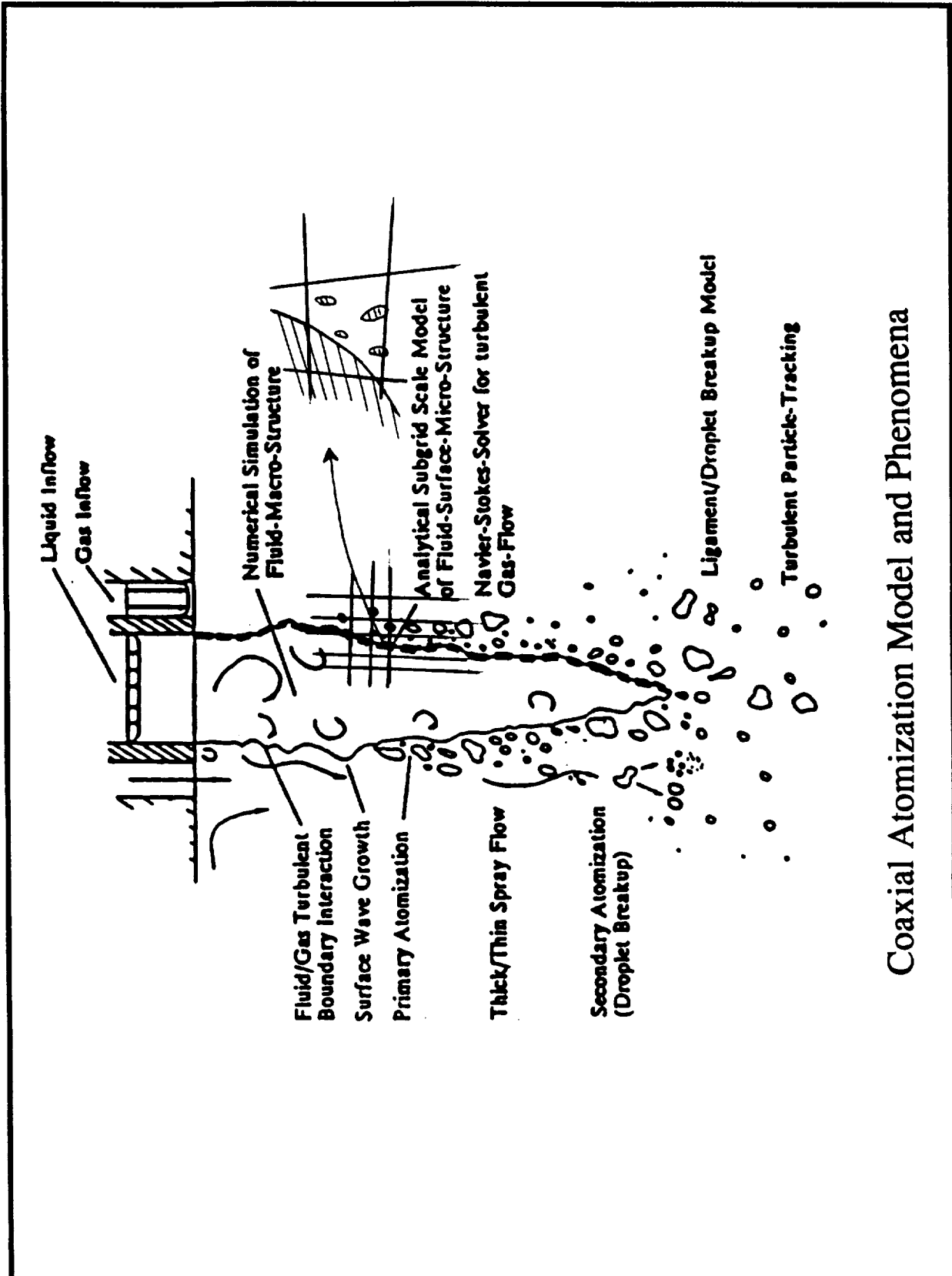
**Y.S.Chen
Engineering Sciences Inc.**

**Workshop for CFD Application in Rocket Propulsion
April 20 - 22, 1993**

NASA/Marshall Space Flight Center.

INTRODUCTION.

- o The dense and dilute spray combustion in liquid rocket engine.
- o The onset of cavitation occurring in swirl injection elements used in STME.
- o The atomization processes in shear-induced injector(co-axial) and impinging injector elements.



Coaxial Atomization Model and Phenomena



Enlarged Picture of a Liquid jet from X-ray Image

OBJECTIVES.

- o To improve the analytical capability for predicting spray combustion processes in liquid-rocket engine.
- o To develop efficient methodologies for spray combustion simulation.
 - Droplet Dispersion.
 - Dilute and Dense Spray.
 - Atomization.
- o To understand and study liquid-gas interfacial phenomena in liquid rocket propulsion.

METHODOLOGY.

- o A strongly-coupled method has been developed to include the Lagrangian -Tracking scheme into a pressure-velocity coupling algorithm.
- o Non-iterative PISOC Algorithm.
- o Easy to include physical models.
 - Evaporation
 - Turbulence
 - Collision and Breakup
 - Finite Rate Chemistry
- o Avoid global iteration between two phase.
- o Time accurate after prescribed corrector steps
- o Using VOF method (volume of fraction) to define and track the liquid-gas interfaces

APPROACHES.

- o Stochastic Particle Tracking Technique
 - Stochastic separated flow(SSF) model.
 - Parcel PDF transport model.
- o Incorporation of Dense Spray effects.
 - Taylor analogy breakup(TAB) model.
 - Reitz's wave instability model.
 - Droplet collision and coalescence model.
- o Eulerian-Lagrangian Frame.
- o Atomization Model.
 - Blob Injection.
 - Volume of Fluid Method.

SHARP SURFACE BETWEEN TWO FLUIDS.

o Eulerian Volume of Fraction Method.

o VOF Equation.

$$\frac{\partial F}{\partial t} + \bar{V} \Delta_i F = 0$$

$$F(\bar{x},t) = \begin{cases} \text{if } F=0.0 & \text{Gas} \\ \text{if } 0 < F < 1.0 & \text{Free Surface} \\ \text{if } F=1.0 & \text{Liquid} \end{cases}$$

o Chakravarthy & Osher High Order Upwind Scheme.

SURFACE TENSION EFFECT.

- o Continuous Surface Force Procedure Used.
- o Surface Tension treated as a limiting Body Force F_{sv} included in the momentum equation.
- o Avoid Jump Conditions in Pressure corrections.
- o Efficient.
- o F_{sv} has to be calculated accurately.

$$F_{sv}(x) = \sigma \kappa(x) \Delta_i F(x) / [F]$$

σ : Surface tension coefficient

κ : Free surface curvature

Two-Way Coupling Scheme

- Predictor Step

- Solve Momentum Implicitly Including Two-Way Coupling Term,

$$\left(\frac{\rho^{n-1}}{\Delta t} + A_p\right)U_i^* = H'(U_i^*) - \Delta_i p^n + S_{ui} + \frac{\rho^{n-1}U_i^n}{\Delta t} - S_p^n U_i^* + R_p^n$$

- Activate Droplet Injection, Evaporation, Breakup and Collision
- Update Particle Velocity v_i^* and Relaxation Time τ^*

$$v_i^* = \frac{v_i^n + (U_i^* + u_i' + F_{bi}^n)\frac{\Delta t}{\tau^n}}{1 + \frac{\Delta t}{\tau^n}}$$

- Evaluate Two-Way Coupling Terms, S_p^* , R_p^* , S_{ml} , and S_{hl}

• **First Corrector Step**

– **Momentum Equation is Approximated by**

$$\left(\frac{\rho^{n-1}}{\Delta t} + A_p\right)U_i^{**} = H'(U_i^*) - \Delta_i p^* + S_i + \frac{\rho^{n-1}U_i^n}{\Delta t} - S_p^*U_i^{**} + R_p^*$$

– **Subtracted to Predictor Equation and Get New Velocity**

$$U_i^{**} = U_i^* - D_u^* \Delta_i (p^* - p^n) - D_u^* [(S_p^* - S_p^n)U_i^* - (R_p^* - R_p^n)]$$

$$D_u^* = \left(\frac{\rho^n}{\Delta t} + A_p + S_p^*\right)^{-1}$$

– **Substitute into Continuity Equation and Obtain Pressure Correction Equation**

$$\left[\frac{1}{\Delta t RT^*} + \Delta_i \left(\frac{U_i^*}{RT^*}\right) - \Delta_i (\rho^{nT} D_u^* \Delta_i)\right] (P^* - P^n) = - \left[\frac{\rho^{nT} - \rho^n}{\Delta t} + \Delta_i (\rho^{nT} U_i^*) \right] + S_{m,i} + \Delta_i \{ \rho^{nT} D_u^* [(S_p^* - S_p^n)U_i^* - (R_{pi}^* - R_{pi}^n)] \}$$

First Corrector Step (continued)

- Update Particle Velocity v_i^{**} and Relaxation Time τ^{**}

$$v_i^{**} = \frac{v_i^n + (U_i^{**} + u_i' + F_{bi}\tau^*)\frac{\Delta t}{\tau}}{1 + \frac{\Delta t}{\tau}}$$

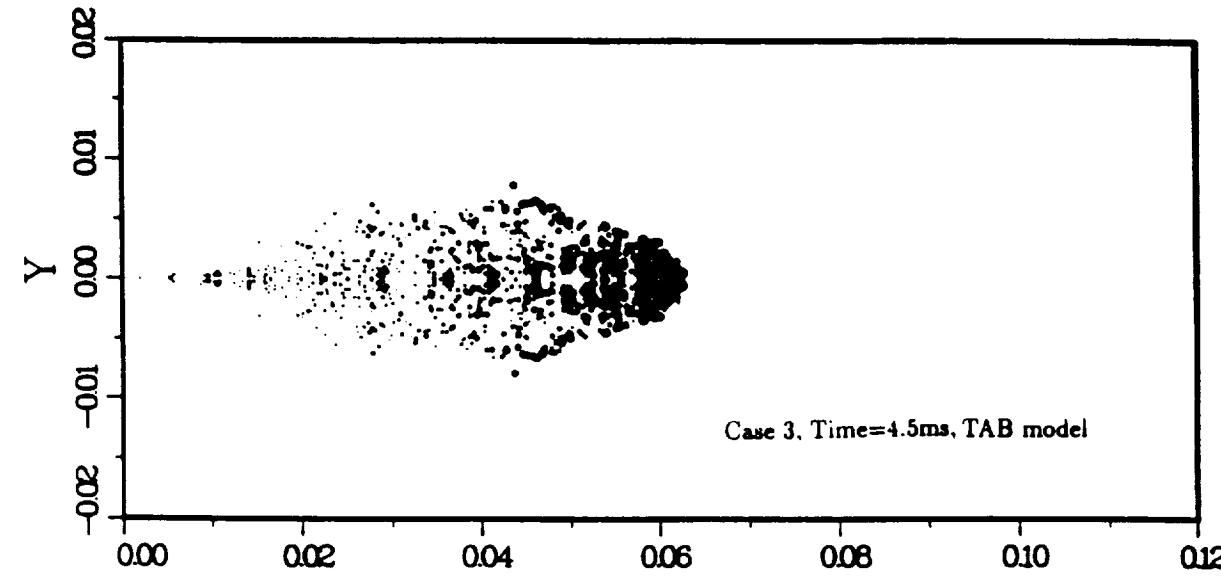
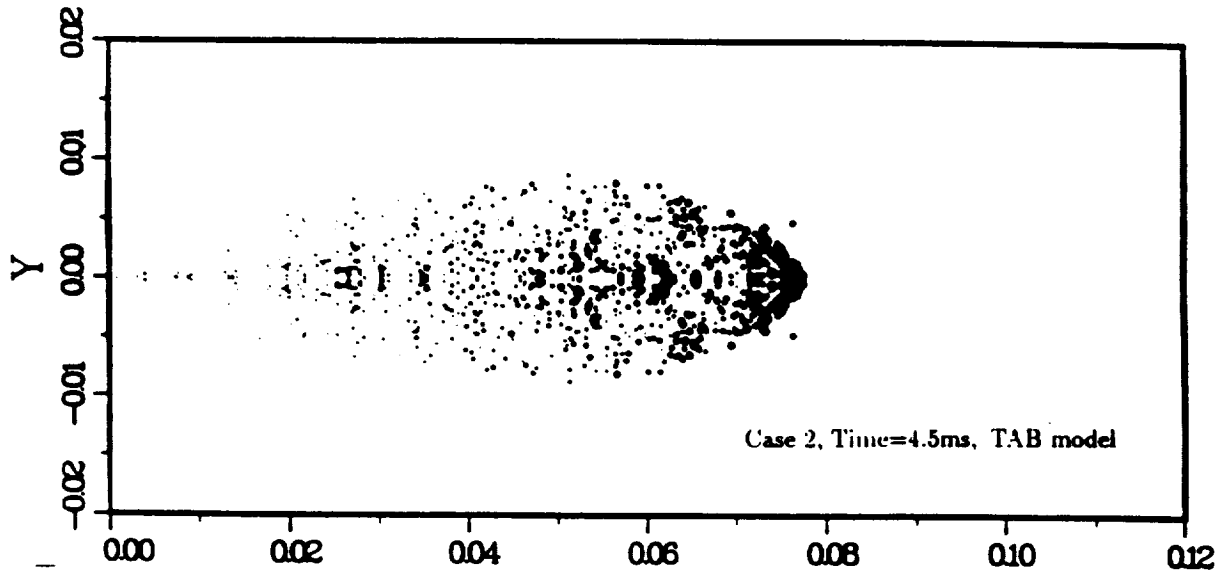
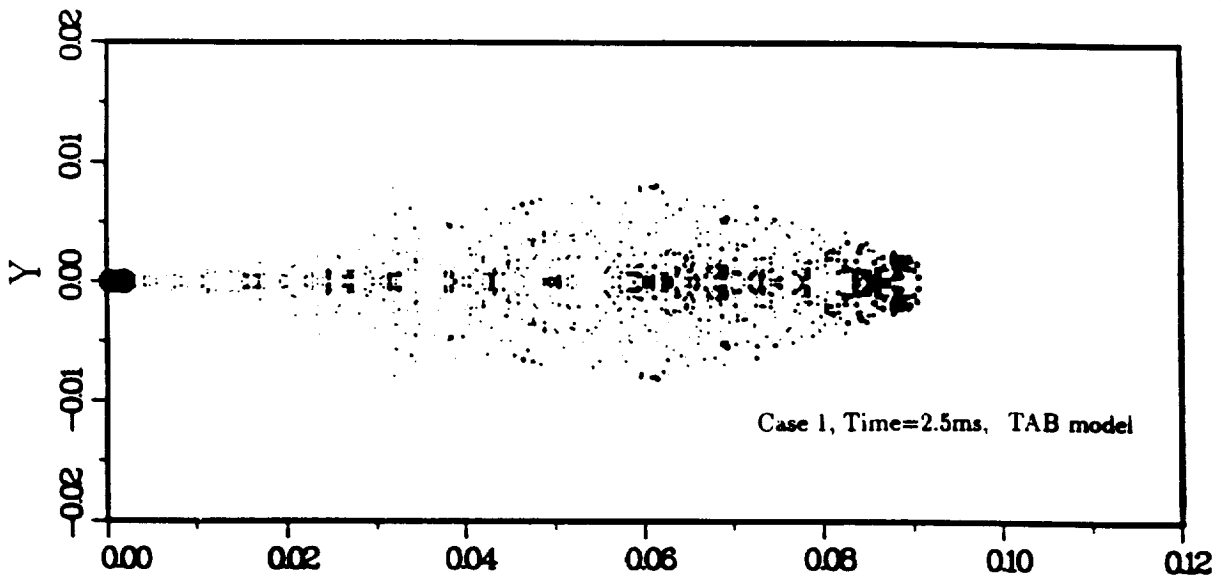
- Evaluate S_p^{**} and R_p^{**} .
- Mean Velocity Field Satisfies the Continuity Constraint.

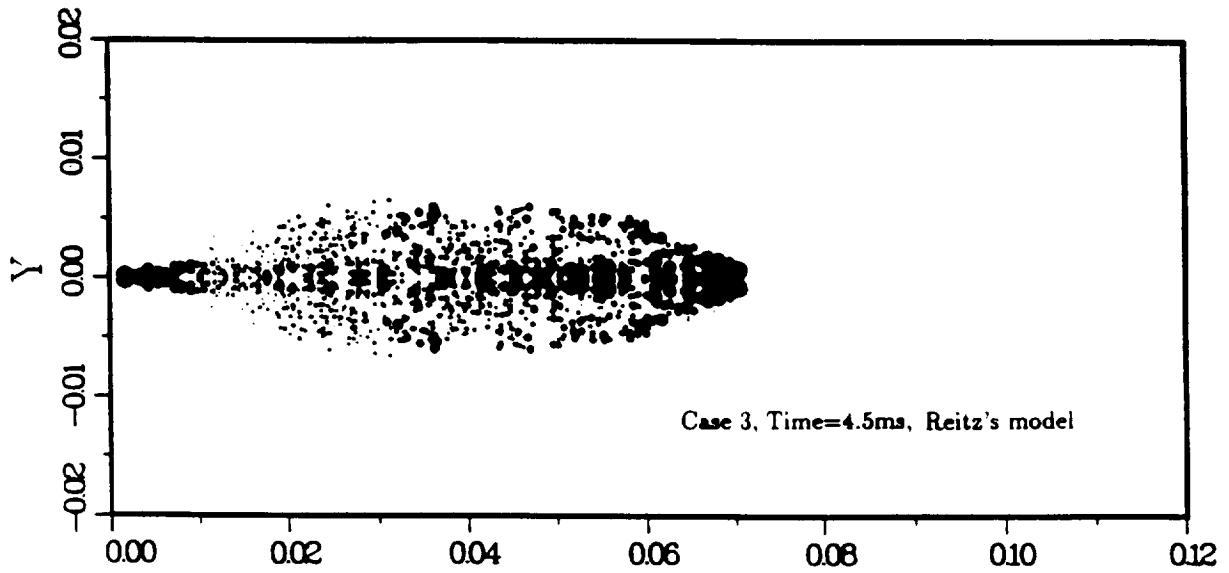
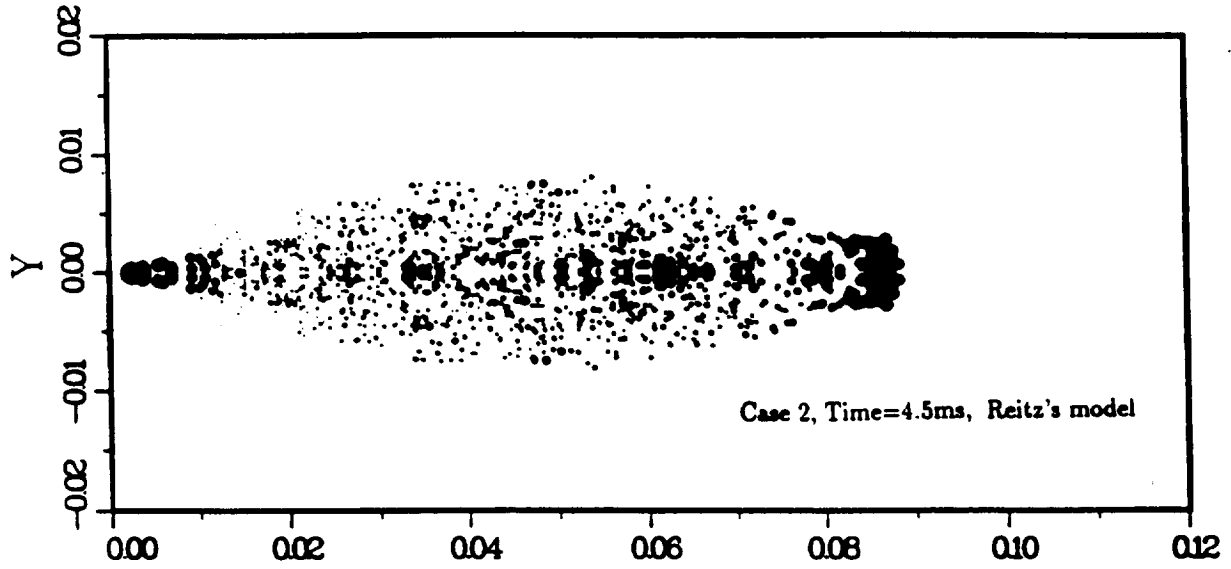
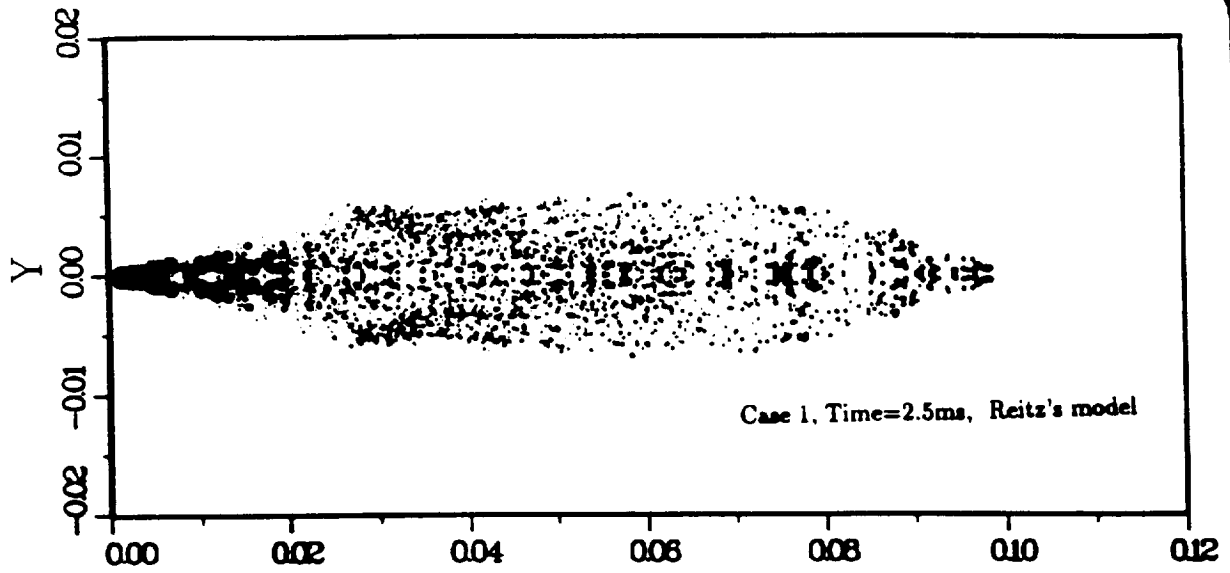
VALIDATIONS & APPLICATIONS.

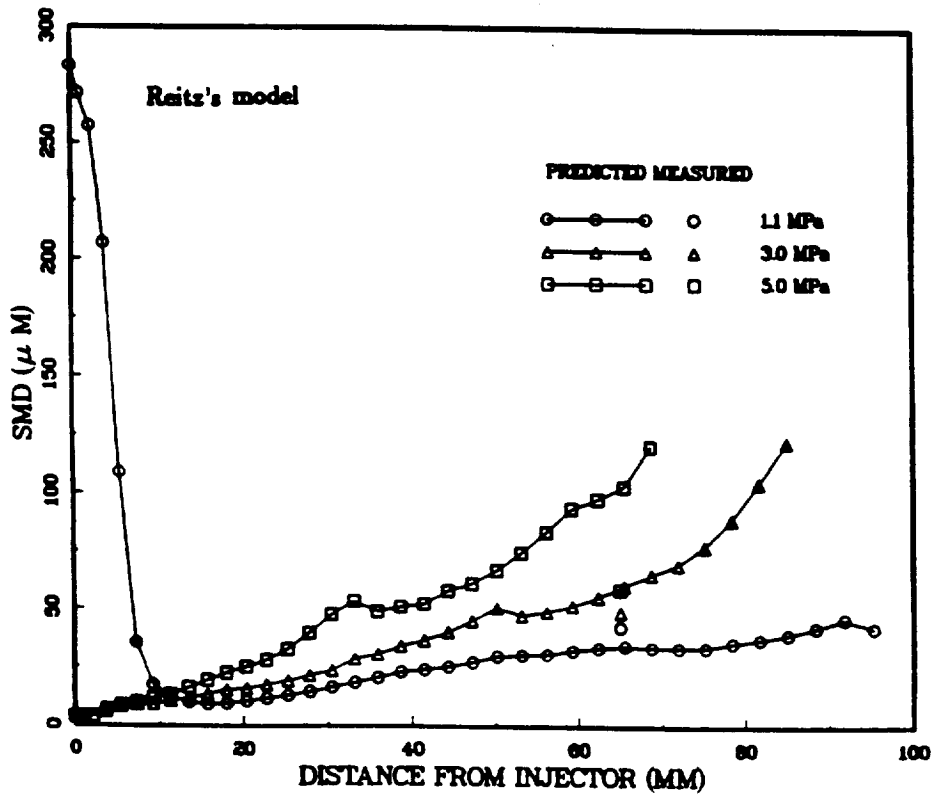
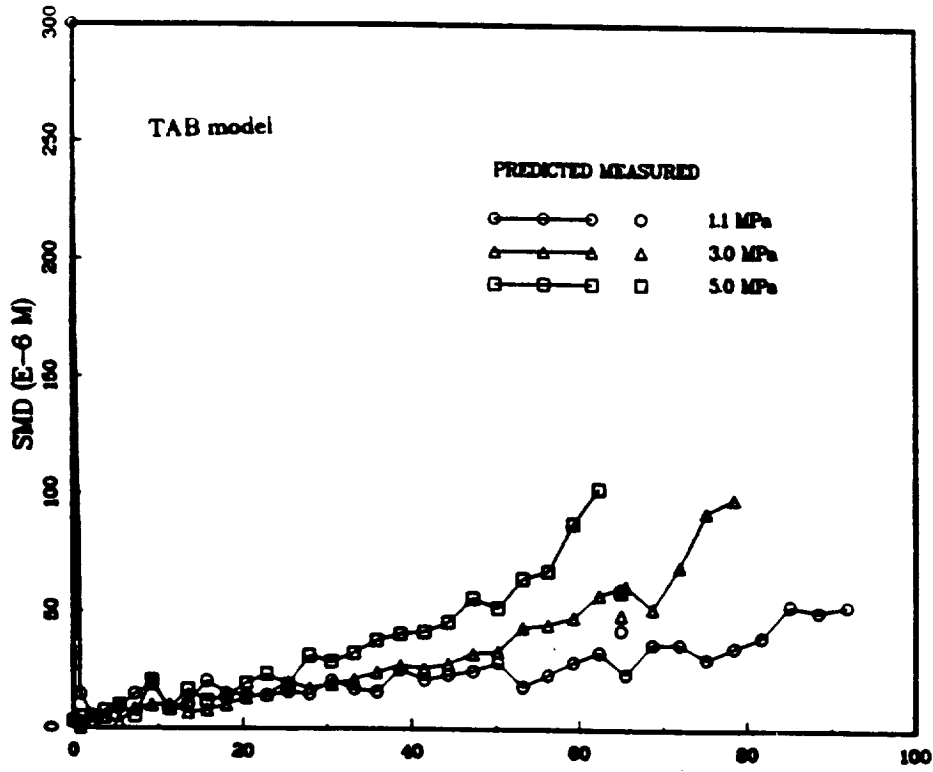
- o Particle Dispersion.
- o Non -evaporating Hollow-Cone Spray.
- o Gas-Droplet round Jets.
- o Non -evaporating and Evaporating Single Jet.
- o Evaporating and Burning solid-Cone Spray.
- o Liquid Column Instability Problem.
- o Droplet Breakup Problem.

o Non- Evaporating Transient Solid-cone Spray.

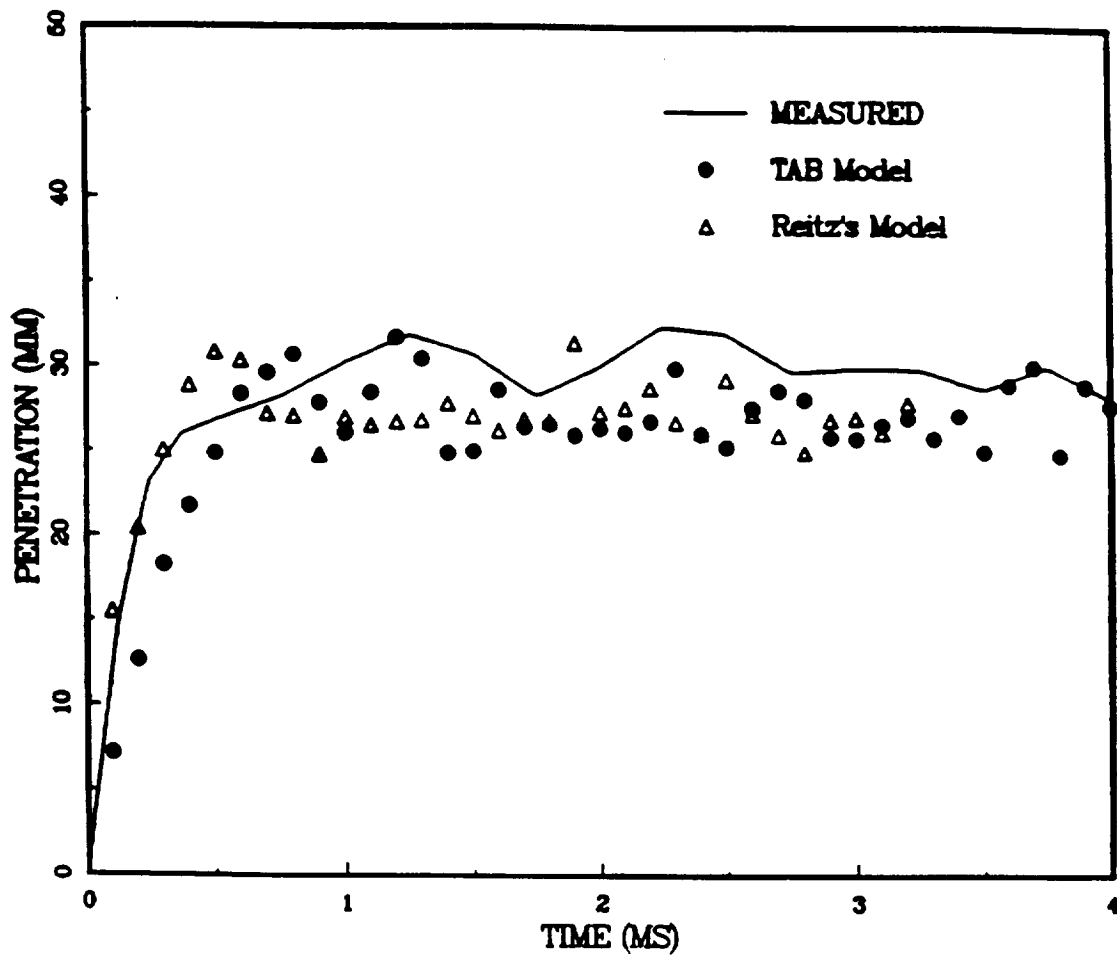
- o Measurements of Hiroyasu and Kadota.
- o Liquid jet injected into high pressure chamber.
- o Transient Flow.
- o To compare jet penetration length and droplet size.
 - Nozzle diameter : 300 μ m
 - Injection pressure : 9.9 MPa
 - Liquid fuel : diesel







Sauter mean diameter ver. distance from the injector



Spray tip penetration ver. time in an evaporating spray

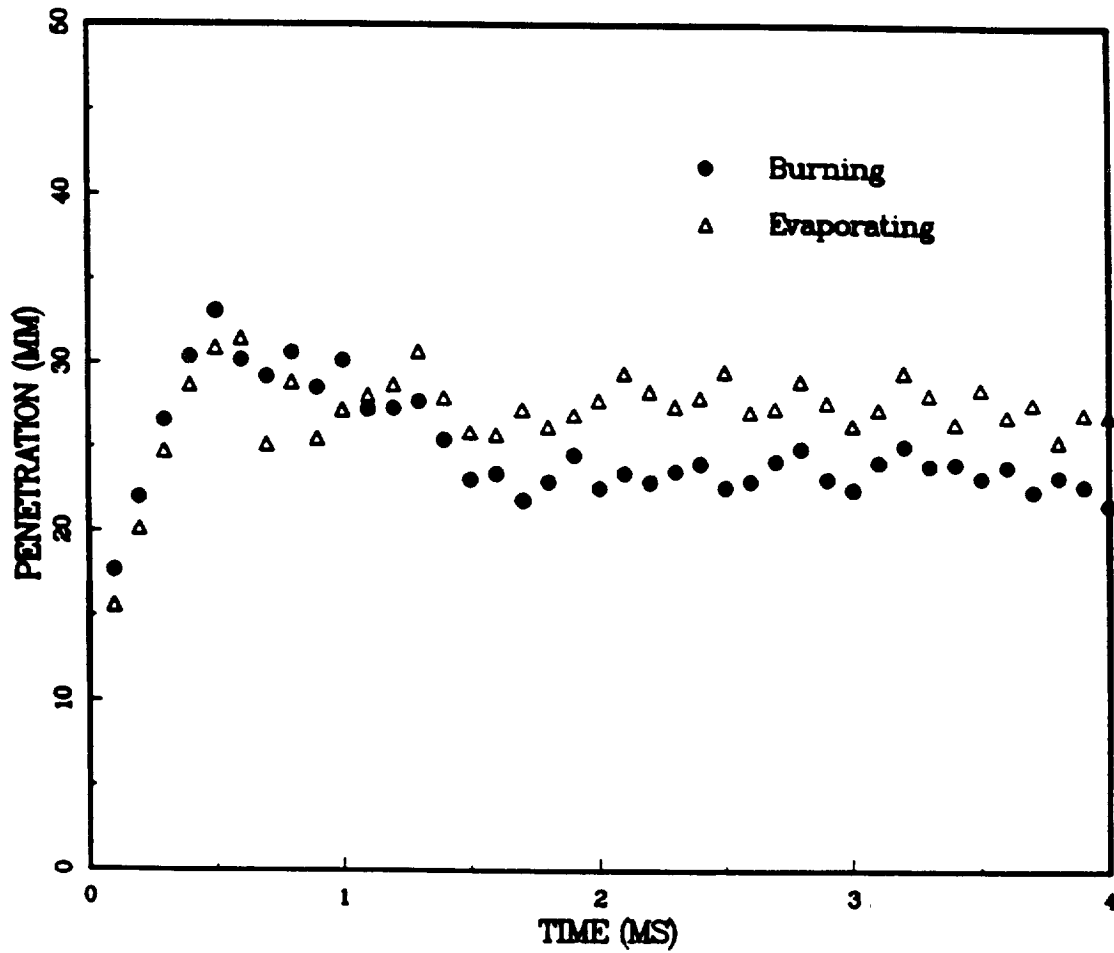
o Evaporating and Burning Solid-Cone Spray.

- o Measurement of Yokota et al.
- o Liquid fuel (tridecane) injected into high pressure, high temperature nitrogen or air.
- o Dense spray and turbulent.
- o Liquid jet atomization and droplet secondary breakup.
- o Single step chemical reaction .



Test Conditions for the Measurement of Yokota et al.

Case	Pinj (MPa)	Pgas (MPa)	Tamb (K)	Minj (kg/s)	Atmosphere
Evaporating Spray	30	3.0	900	0.00326	<i>N₂</i>
Burning Spray	30	3.0	900	0.00326	<i>Air</i>



Comparison of penetration length ver. time for burning and evaporating sprays

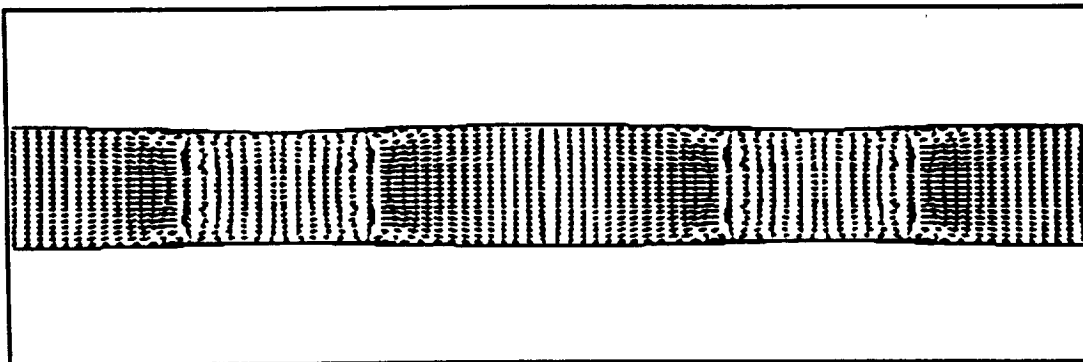
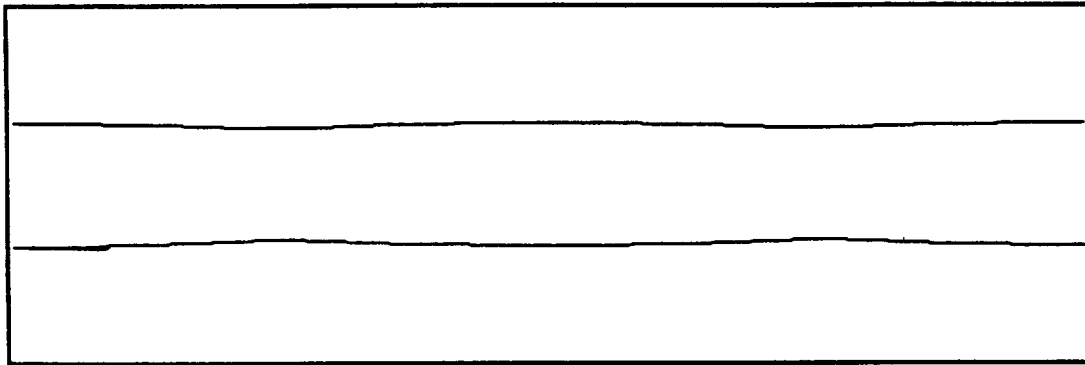
o Liquid Column Instability Problem.

o Cylindrical Liquid Column.

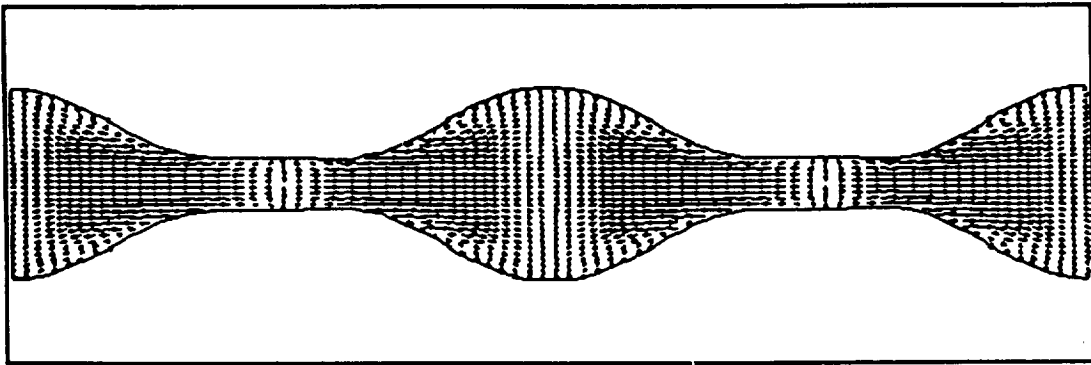
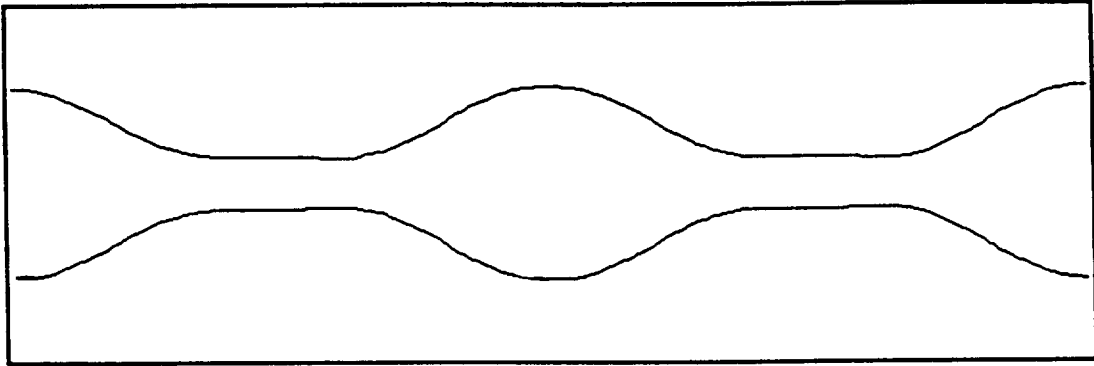
- density : 1g/cm^3
- surface tension coefficient : 72.8 dyne/cm
- diameter : 0.1 cm
- length : 1 cm

o Initial perturbation.

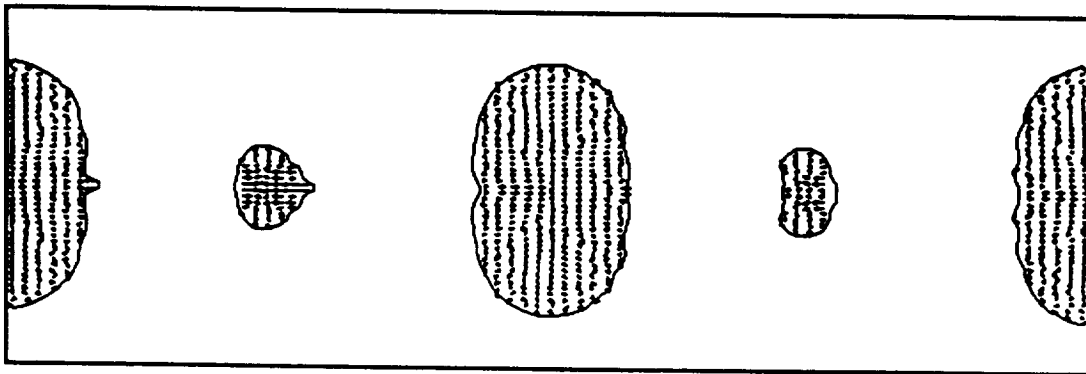
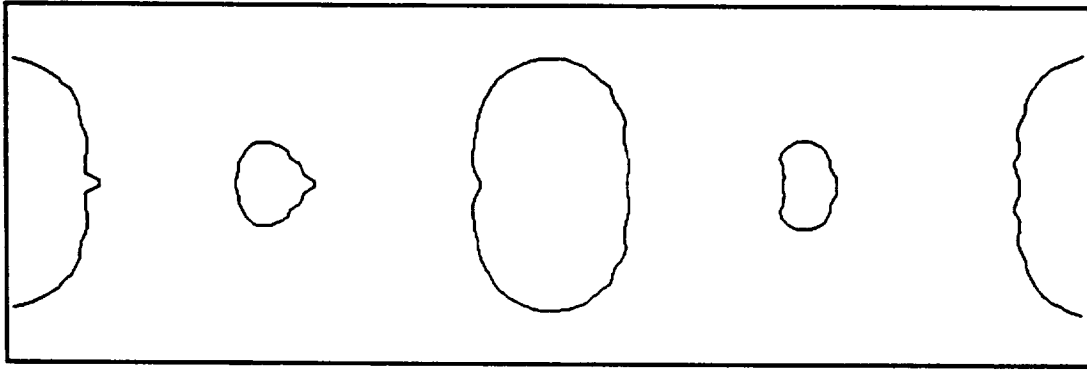
$$0.001 \cdot R_0 \cdot \text{COS}(\pi x/L)$$



Liquid Column Jet Breakup Problem
Time = 2.501×10^{-2} sec Cycle= 1114
(a) Surface
(b) Velocity vector



Liquid Column Jet Breakup Problem
Time = 3.700×10^{-2} sec Cycle= 1647
(a) Surface
(b) Velocity vector



Liquid Column Jet Breakup Problem
Time = 4.002×10^{-2} sec Cycle = 1813
(a) Surface
(b) Velocity vector

o Liquid Droplet Breakup

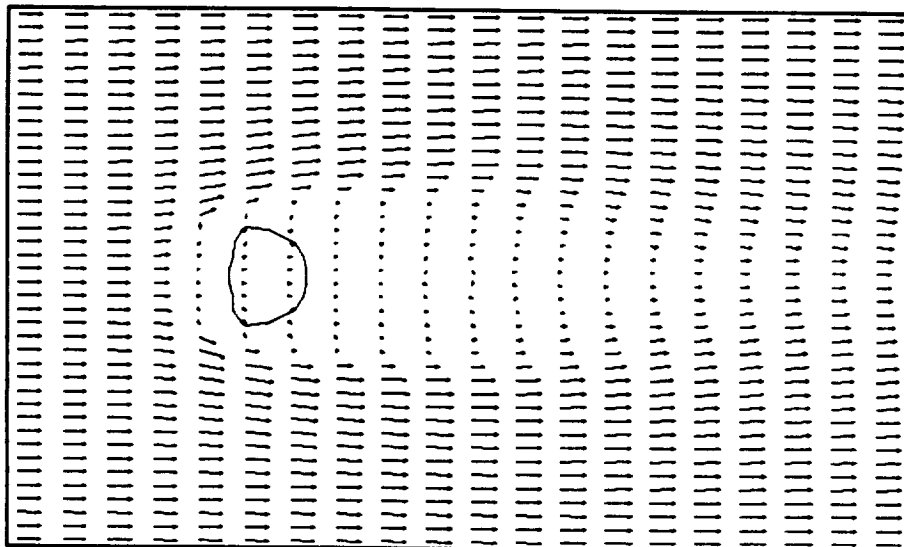
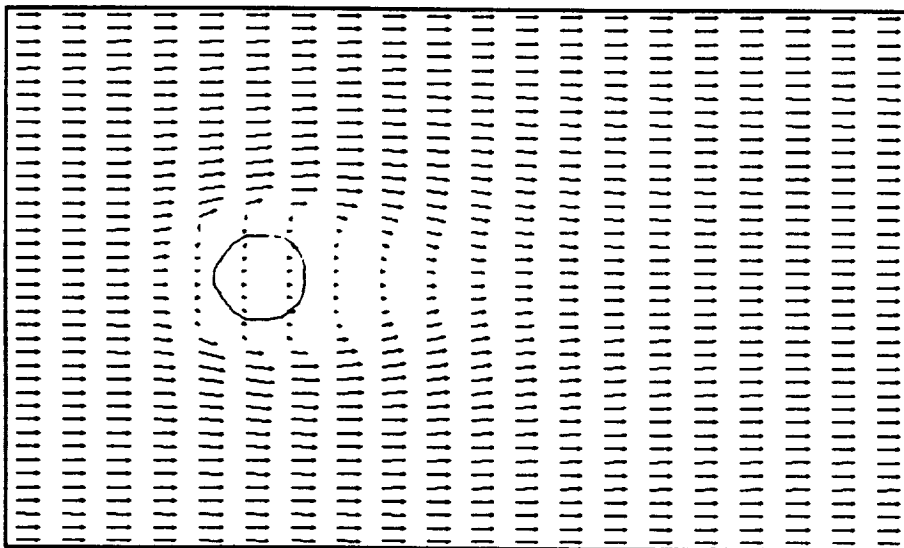
o Liquid (Kerosene)

- density : 1g/cm^3
- surface tension coefficient : 30.0 dyne/cm
- viscosity : 0.018 poise
- initial radius : $125\text{ }\mu\text{m}$

o Gas (air)

- density : 1g/cm^3
- viscosity : 0.0018 poise
- initial velocity : 10000 cm/sec

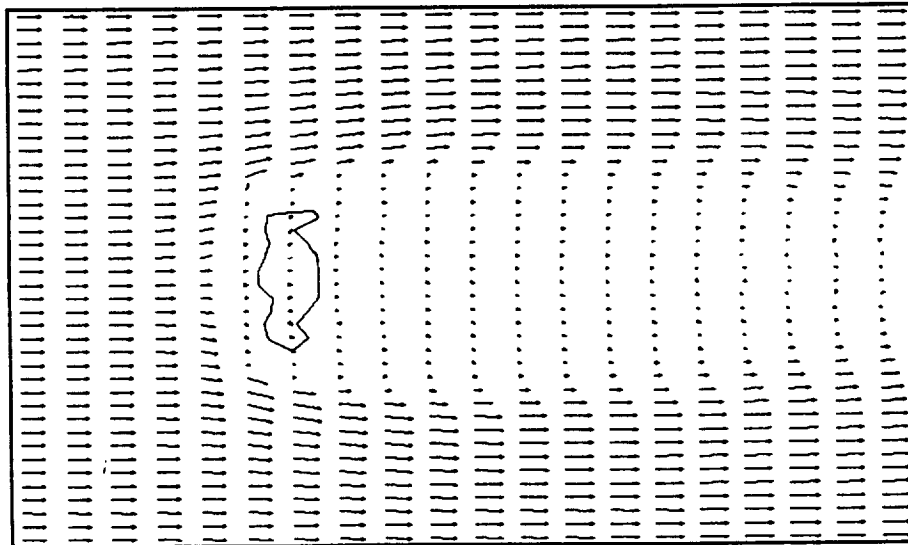
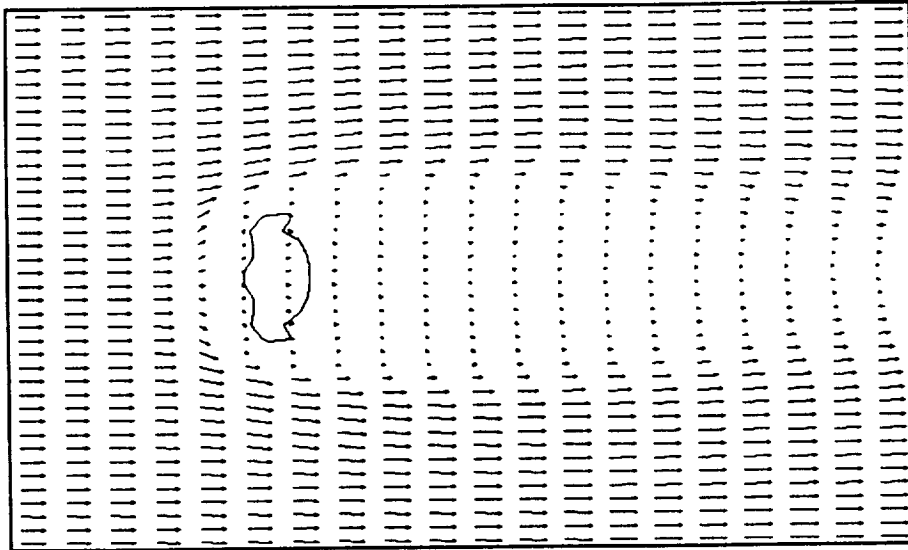
o Physical domain : $1.25\text{cm} \times 0.15\text{cm}$



Liquid Droplet Breakup Problem

(a) Time = 4.078×10^{-6} sec Cycle= 26

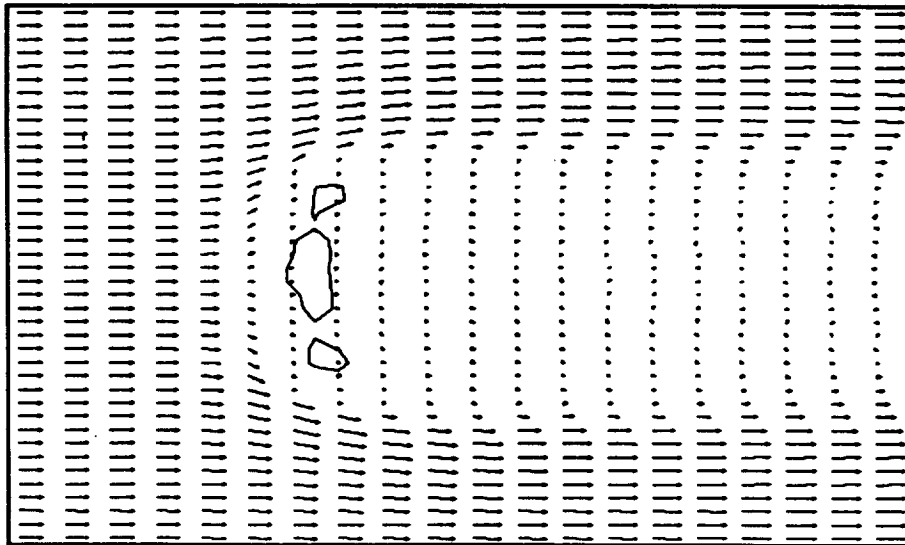
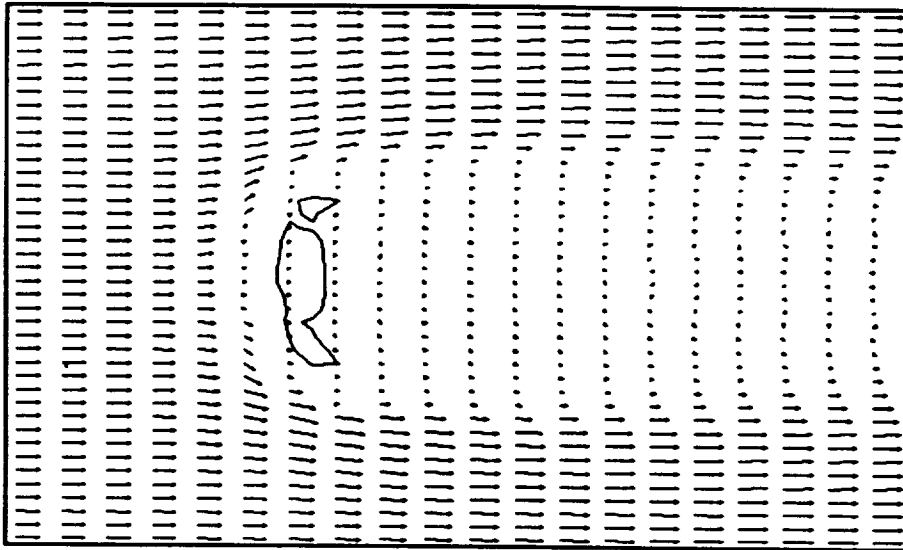
(b) Time = 1.909×10^{-5} sec Cycle= 123



Liquid Droplet Breakup Problem

(a) Time = 3.410×10^{-5} sec Cycle= 219

(b) Time = 4.401×10^{-5} sec Cycle= 284



Liquid Droplet Breakup Problem

(a) Time = 5.409×10^{-5} sec Cycle= 351

(b) Time = 5.911×10^{-5} sec Cycle= 385

CONCLUSION AND WORK IN PROGRESS

- o Preliminary Implementation of VOF in successful.
- o Turbulence Effects will be included soon.
- o Compressibility Effects is currently incorporated in the Gas Phase.
- o Incorporation of other physical Submodels.

