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MODELING OF NON-SPHERICAL DROPLET DYNAMICS

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ABSTRACT

A two-dimensional time-dependent computer code based on the modified Arbitrary Lagrangian Eulerian(ALE) technique has been developed to simulate non-spherical droplet dynamics and evaporation under convective flows at real rocket combustion chamber conditions. The equations of mass, momentum, energy and species are simultaneously solved for both liquid and gas phases with an accurate dynamic interface tracking. The jump boundary conditions across the deforming droplet surface are obtained by applying the integral forms of conservation of mass, momentum, and energy. At each time step, the interface geometry and flow properties at the droplet surface are implicitly solved by satisfying the interface boundary conditions. A Lagrangian technique was developed to track the arbitrarily moving interface between the liquid droplet and the external gas. An elliptic grid generator is adopted to dynamically reconstruct grids both inside and outside the droplet surface.

This code has been used to study droplet oscillation, droplet deformation/breakup, non-spherical droplet evaporation in both low and high pressure convective flows.

This presentation briefly describes the numerical algorithm for modeling of the non-spherical droplet dynamics and demonstrates the representative simulation results of non-spherical droplet evaporation at low and high pressure convective flows. Potential applications of this code to rocket combustor design and performance predictions are discussed.

Modeling of Non-Spherical Droplet Dynamics

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Motivation:

- Droplet dynamics and vaporization process has been assumed to control combustor performance and combustion instability.
- Both experimental and theoretical studies on non-spherical droplet dynamics/combustion at realistic conditions are limited.
- High performance liquid rocket engines operate at chamber pressures exceeding the critical pressure of the propellants.

Objective:

To develop a comprehensive CFD model to predict non-spherical droplet dynamics and evaporation at both low- and high-pressure environments in realistic combustion chamber.

Model Description:

- Time-dependent, two-dimensional, viscous, compressible and/or incompressible flows in laboratory coordinates.
- Dynamic interface tracking and grid reconstruction.
- Two(one) species liquid droplet.
- Two(one) species compressible gas mixture(liquid).
- Surface tension force, heat, mass and momentum transfer across interface.
- Low/High pressure phase equilibrium.
- Modified Arbitrary-Lagrangian-Eulerian numerical method.

Gas-Liquid Interface Conditions:

- **Species concentration:**

$$\dot{m}Y_{gf} - \dot{m}Y_{lf} = \rho_g D \nabla \left(\frac{\rho_{gm}}{\rho_g} \right) \cdot \hat{n}$$

- **Continuity of mass flux:**

$$\rho_g \left(\vec{u}_g - \vec{U} \right) \cdot \hat{n} = \rho_l \left(\vec{u}_l - \vec{U} \right) \cdot \hat{n} = \dot{m}$$

- **Continuity of normal momentum flux:**

$$\dot{m} \left(\vec{u}_g - \vec{u}_l \right) \cdot \hat{n} = \left(P_g - P_l \right) \hat{n} - \tau_{gn} \cdot \hat{n} + \tau_{ln} \cdot \hat{n}$$

- **Continuity of energy flux:**

$$\dot{m} \left(E_g - E_l \right) = -\vec{u}_g \cdot \left(P_g - \tau_g \right) \cdot \hat{n} + \vec{u}_l \cdot \left(P_l - \tau_l \right) \cdot \hat{n} - \vec{J}_g \cdot \hat{n} + \vec{J}_l \cdot \hat{n}$$

Gas-Liquid Interface Conditions (Cont.):

- **Low-Pressure Phase Equilibrium:**
  - **Clausius-Chapeyon vapor pressure formula.**
  - **Mass fraction based on vapor pressure and molecular weight.**
- **High-pressure Phase equilibrium: Redklich-Kwong equation of state with mixing rules of Chuen and Prausnitz.**

$$T^{(v)} = T^{(l)}, \quad P^{(v)} = P^{(l)}, \quad \phi_i^{(v)} x_i^{(l)} = \phi_i^{(l)} x_i^{(l)}$$

- **Iterative solution of surface temperature T_s, surface mass fraction Y_{gf} and surface pressure P_g, P_l.**

Gas-Liquid Interface Conditions (Cont.):

- **Non-slip conditions:**

$$T_{gm} = T_{lm} = T_s$$

$$u_{gt} = u_{lt}$$

- **Surface pressure jump conditions:**

$$P_l - P_g = \sigma(T_s, Y_i)\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$$

- **Surface tension coefficient $\sigma(T_s, Y_i)$: Model proposed by Brock and Bird.**

- **Radii of curvature at interface – Cubic Spline**

Dynamic Interface Tracking:

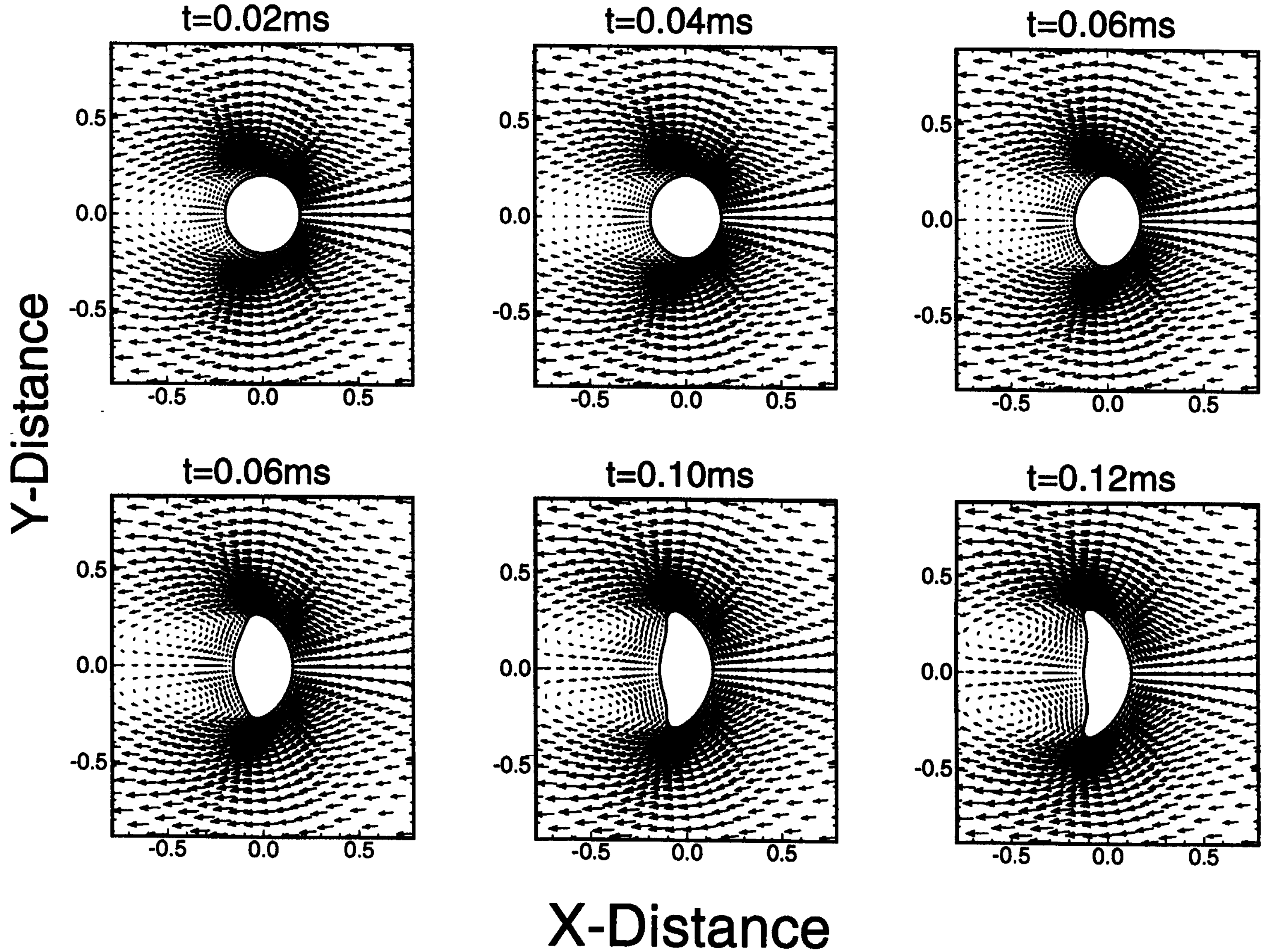
- Dynamic Lagrangian droplet surface tracking.
- Dynamic grid reconstruction based on Poisson Elliptic solver both inside and outside the droplet surface.

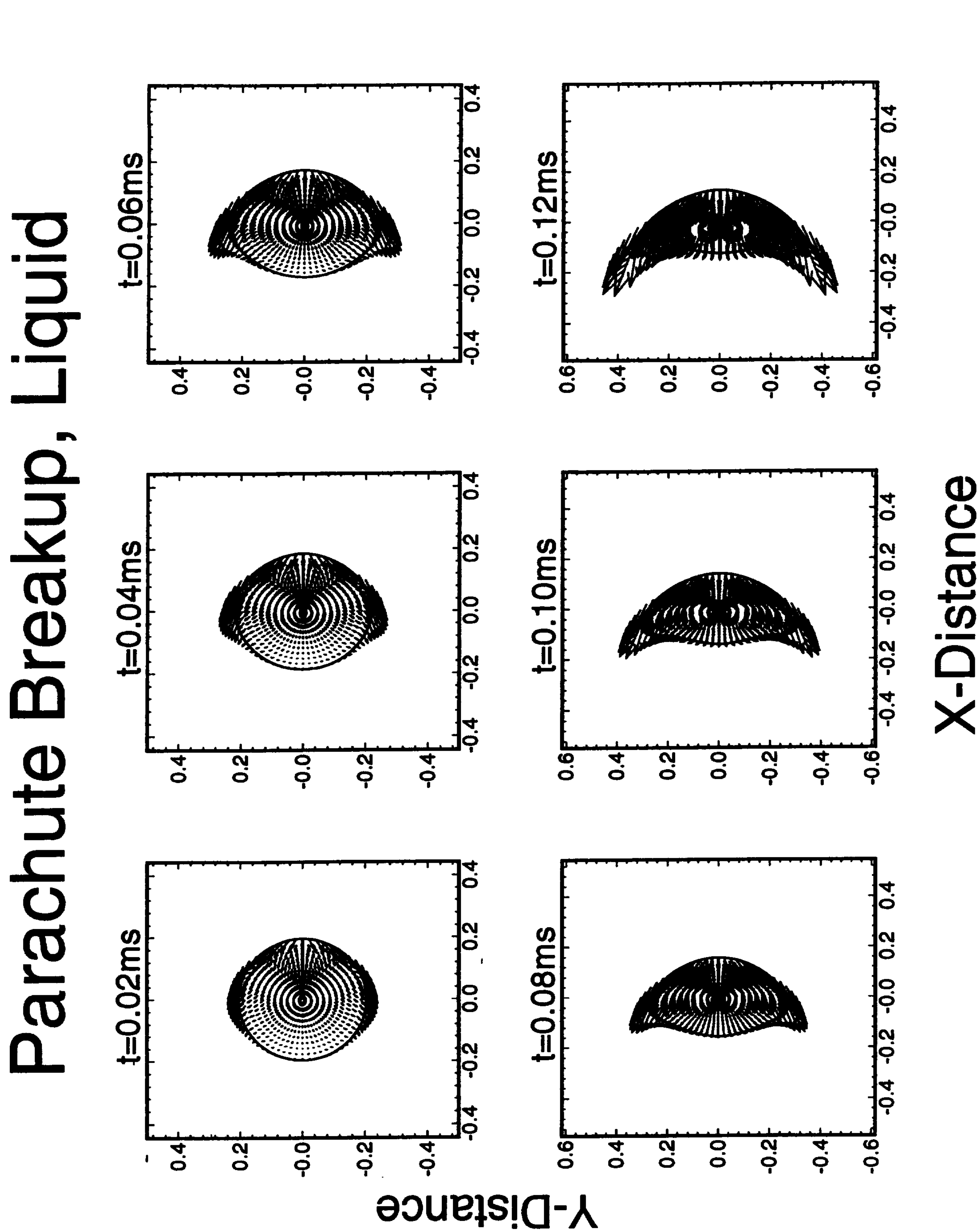
Low-Pressure Droplet Evaporation:

- **N-Heptane fuel, Oxygen gas**
- $P_{amb}/P_{cr} < 1.0$
- $P_{amb} = 1.0\ atm.$
- $W_e R_e^{-0.5} = 1.0$, **Parachute-type breakup.**

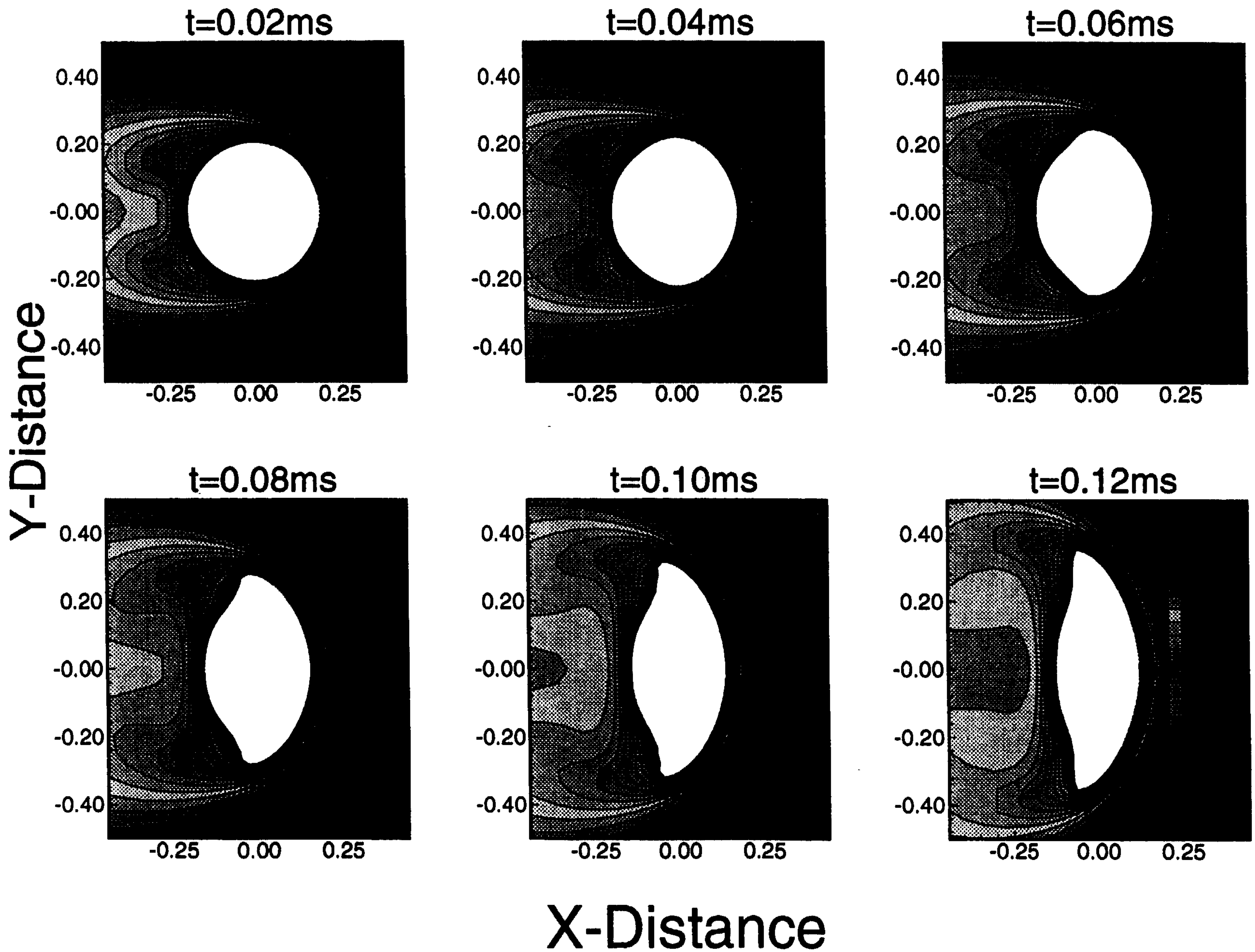
- **Parachute-type,** $8 \leq W_e \leq 40$, $0.2 \leq W_e R_e^{-0.5} \leq 1.6$
- **Striping-type,** $20 \leq W_e \leq 2 \times 10^4$, $1.0 \leq W_e R_e^{-0.5} \leq 20$

Parachute Breakup

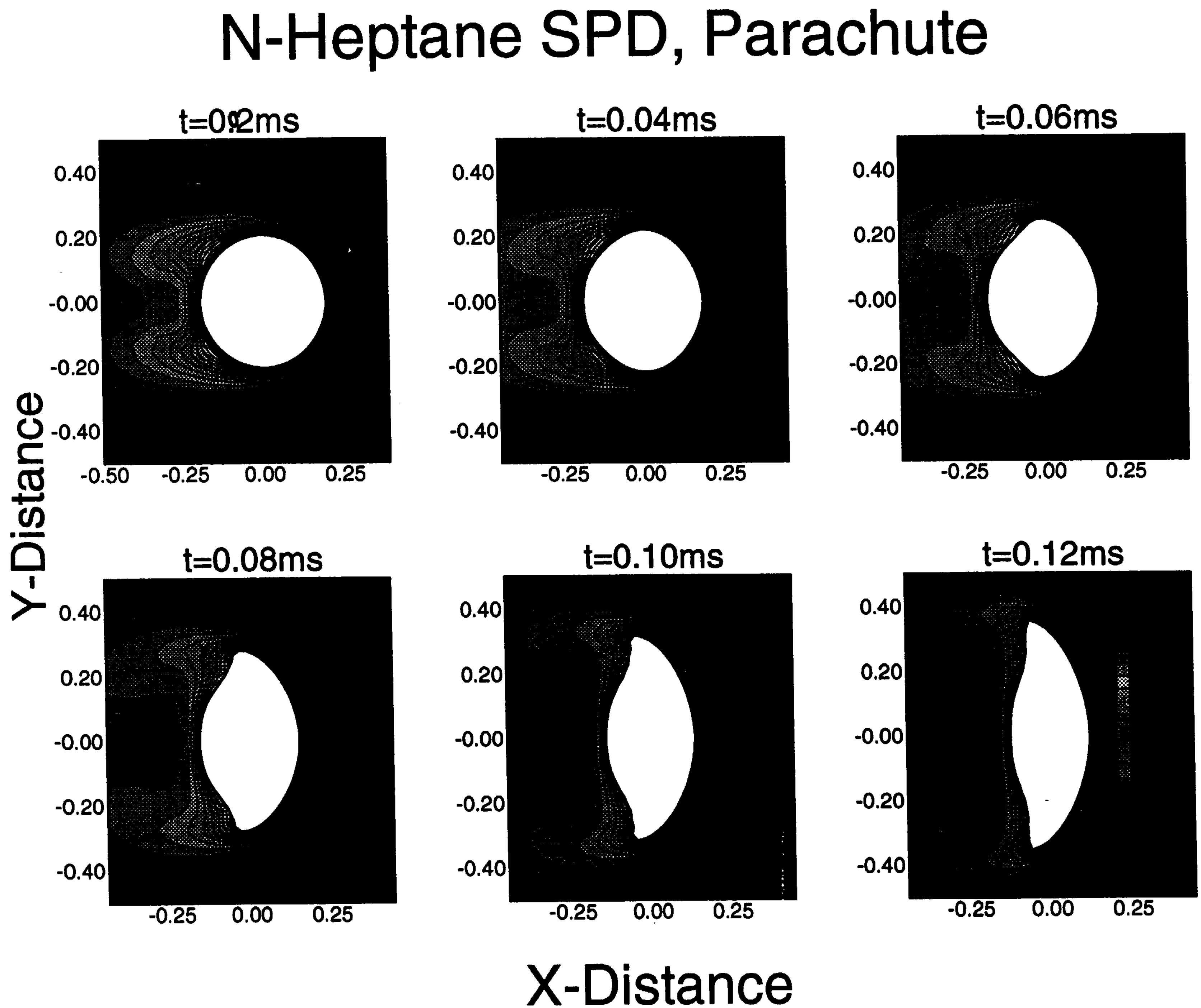


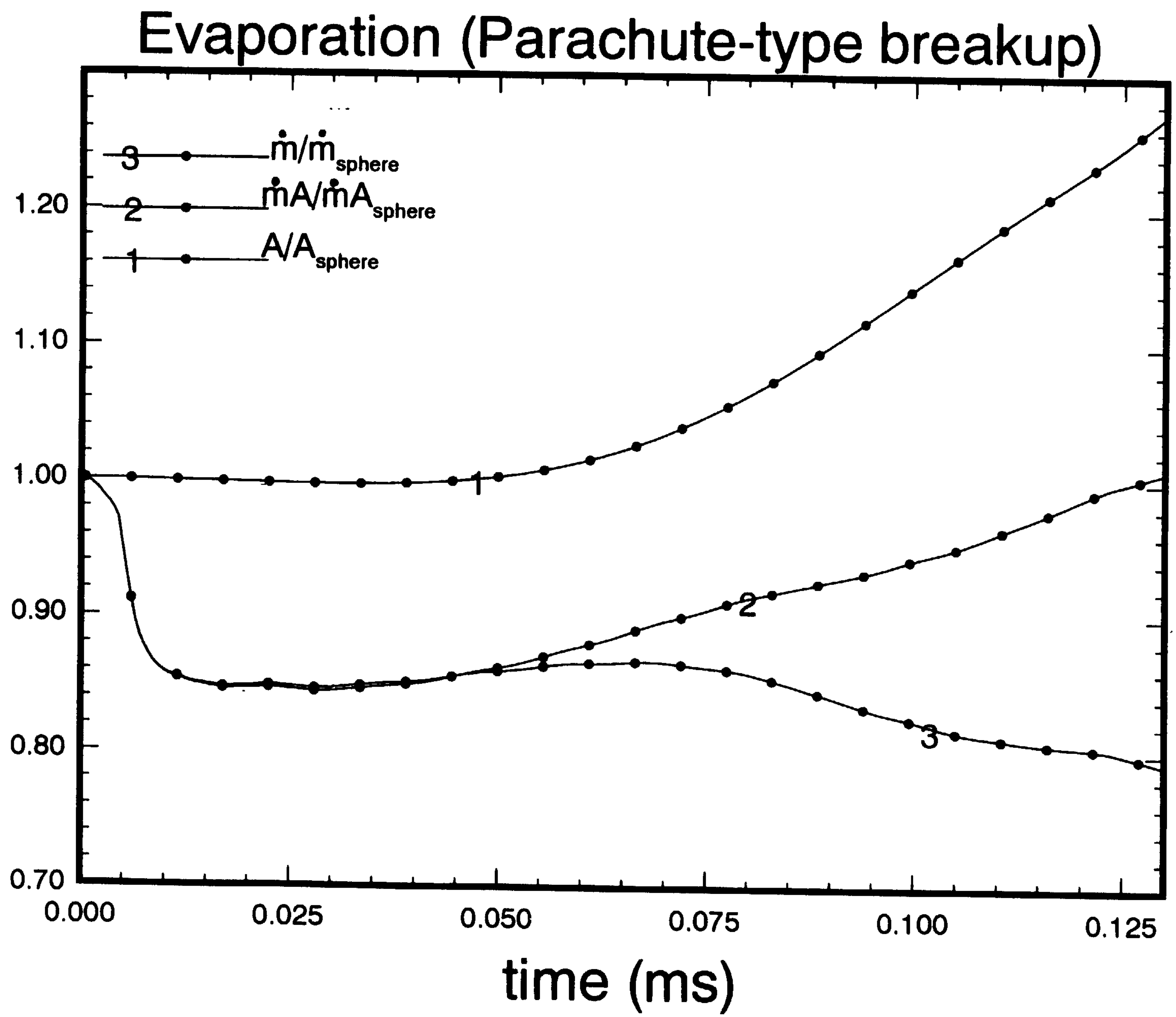

Parachute Breakup, Liquid
t=0.02ms
t=0.04ms
t=0.06ms
t=0.08ms
t=0.10ms
t=0.12ms
X-Distance
Y-Distance

Gas Temperature, Parachute



C-9.

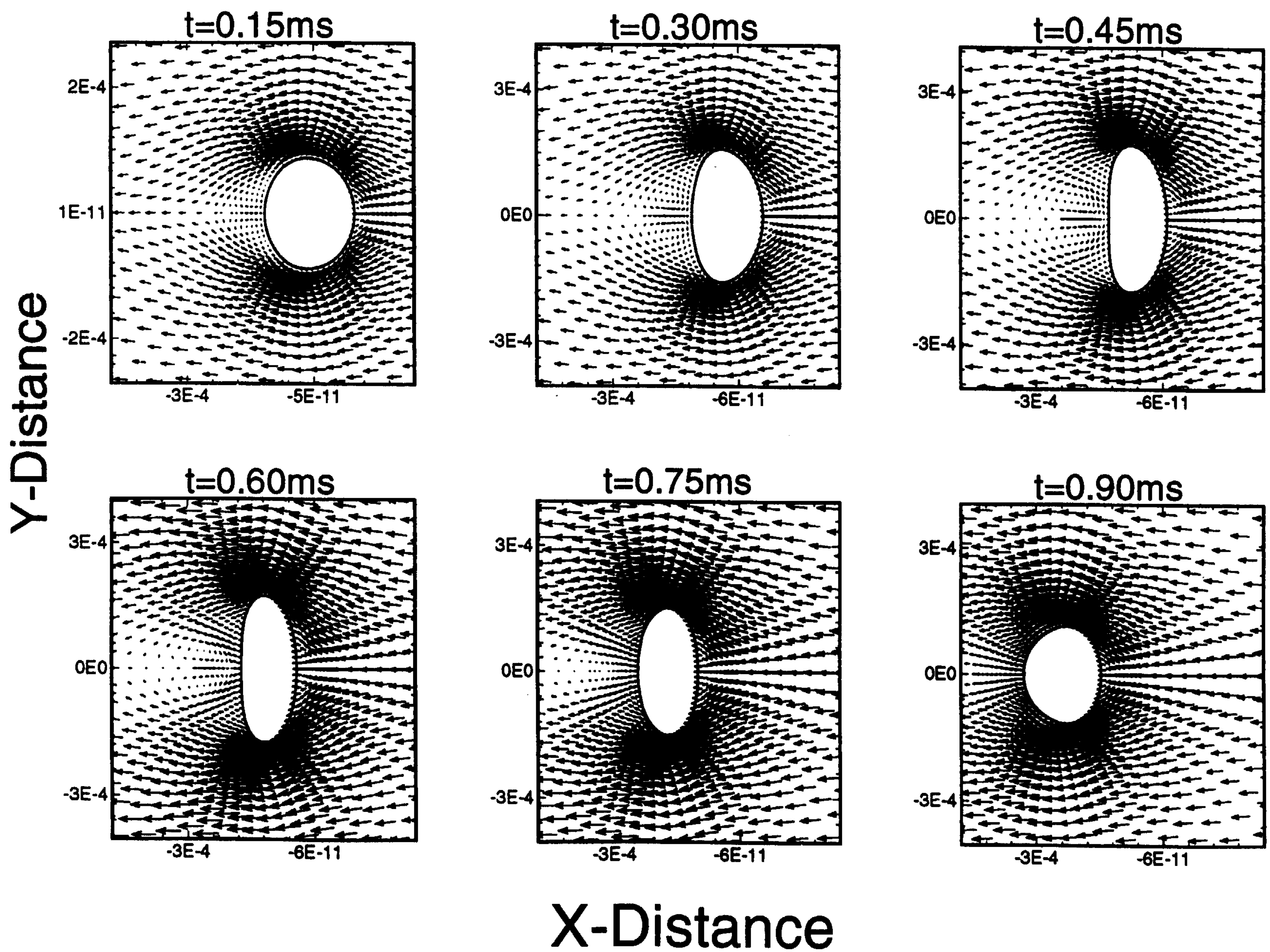

N-Heptane SPD, Parachute
t=0.02ms
t=0.04ms
t=0.06ms
t=0.08ms
t=0.10ms
t=0.12ms
0.40
0.20
-0.00
-0.20
-0.40
-0.50
-0.25
0.00
0.25
Y-Distance
X-Distance


Evaporation (Parachute-type breakup)
3 ṁ/ṁsphere
2 ṁA/ṁAsphere
1 A/Asphere
1.20
1.10
1.00
0.90
0.80
0.70
0.000
0.025
0.050
0.075
0.100
0.125
1
2
3
time (ms)

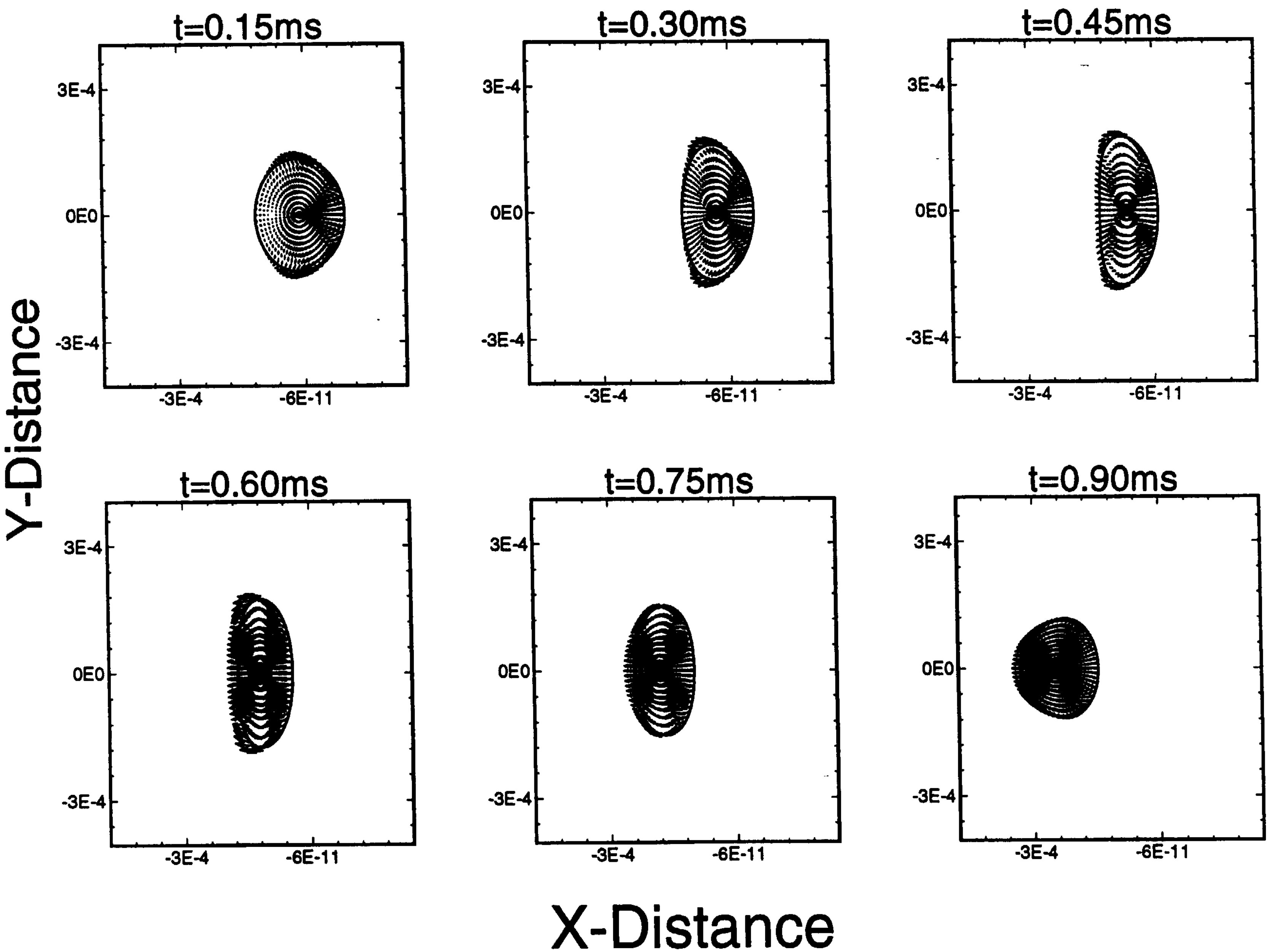
High-Pressure Droplet Evaporation:

- **N-Heptane fuel droplet, hot Nitrogen gas.**
- $T_\infty = 1000K$, $D_0 = 200\mu m$
- $u_\infty = 2, 4, 8\ m/s$. **Oscillation, Bag, Striping.**
- $P_{amb}/P_{cr} = 1.4 > 1.0$, $T_{amb}/T_{cr} = 1.87$
- $P_{amb} = 4.0\ Mpascal$.

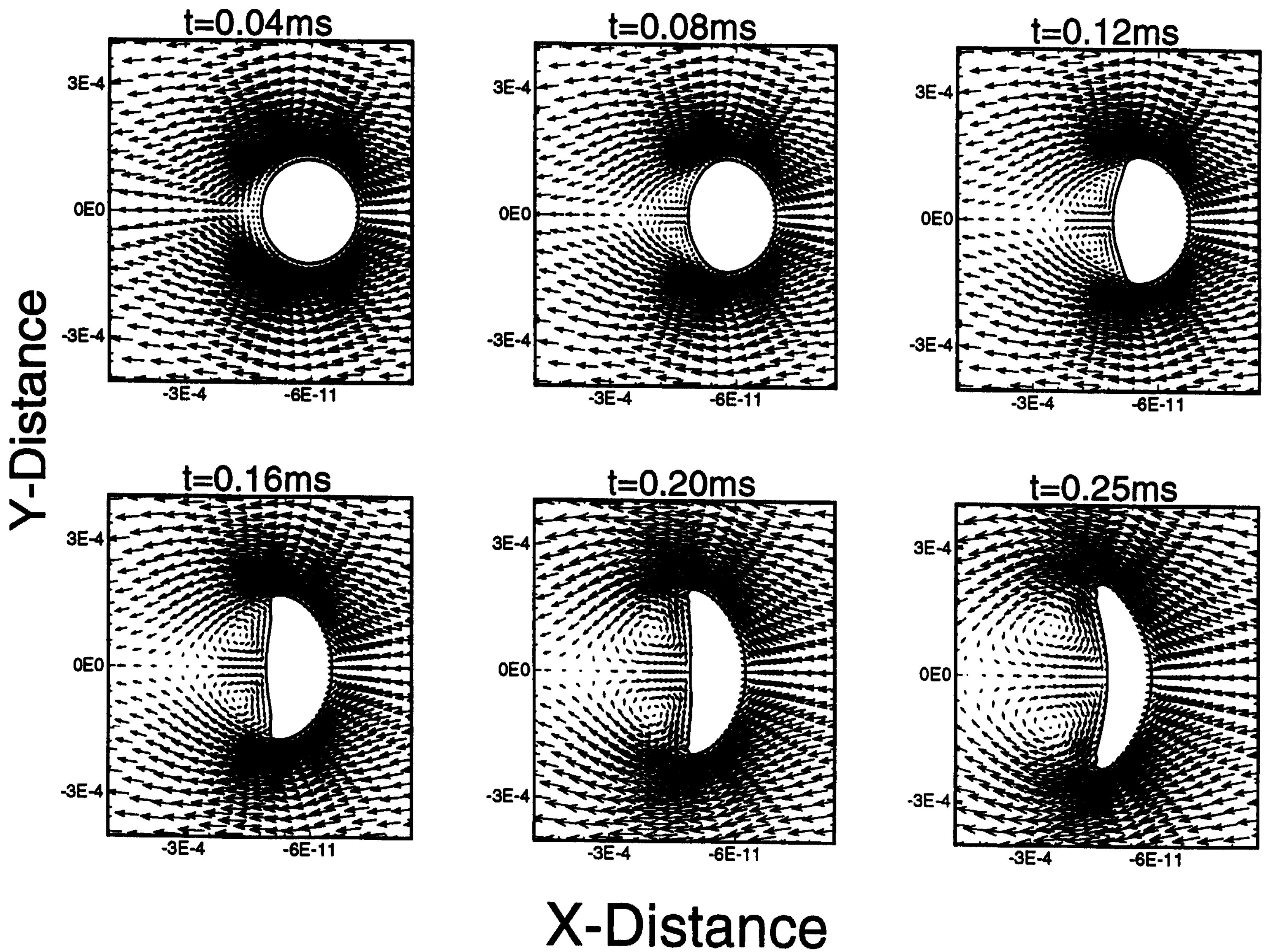
HP, Gas Velocity, 2M/S



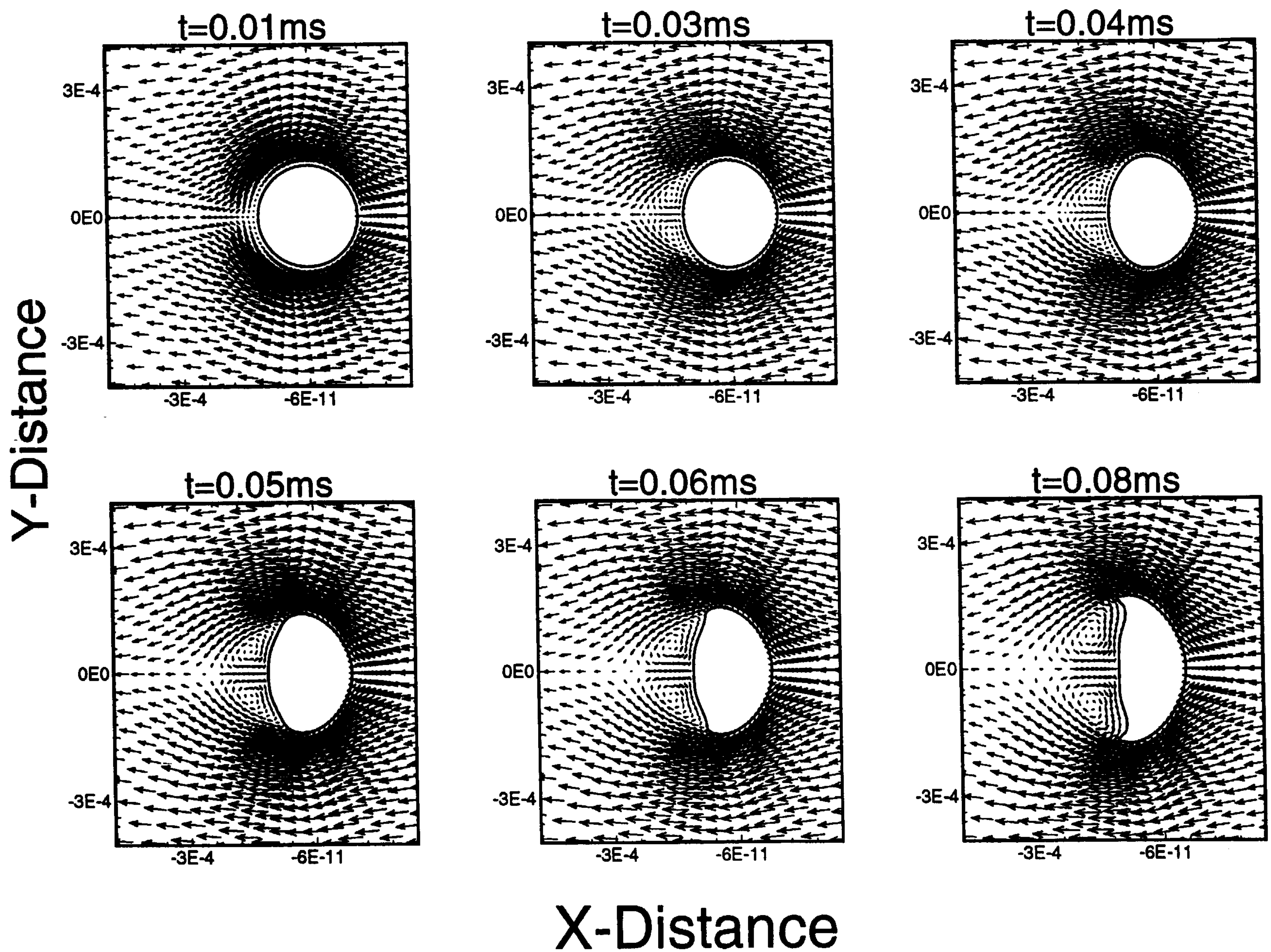
HP, Liquid Velocity, 2M/S



HP, Gas Velocity, 4M/S



HP, Gas Velocity, 8M/s



Conclusions and Recommendations:

- Established a two-dimensional model for non-spherical droplet dynamics and eveporation at both low and high pressure convective environments.
- Breakup is sensitive to gas relative velocity; insensitive to gas temperature.
- Fast engineering correlation to predict droplet behavior can be developed based on this model. Combined with available experimental data, a useful package can be provided for rocket engine combustor design.