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Spray Formation: Three-Dimensional Liquid Break-up due to Surface Tension

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The growth of instabilities on the interface between a liquid jet and its gaseous environment is an important mechanism in spray atomization, and it is the subject of the work reported herein. Numerical simulations based on the Navier-Stokes equations were used to model liquid/gas interface flows. An algorithm was developed for solving the unsteady Navier-Stokes equations for incompressible fluid with a discontinuity in density and with surface tension, and its accuracy was demonstrated. In flows representative of round pressure-atomized jets and pressure-swirl atomizers, nonuniform mean velocity distributions resulting from viscous boundary layers were found to have a significant effect on instability growth. In a round jet, the inclusion of a boundary layer-like velocity profile significantly reduced the growth rate of small wavelength instabilities. The velocity profile had a much greater effect than surface tension on the initial

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atomization process for the flow parameters considered. A good estimate of initial fuel droplet size was obtained by considering boundary layer effects but disregarding surface tension. In a flow representative of the fuel issuing from a pressure-swirl nozzle, nonuniformity of the velocity profile was found to increase the growth rate of a disturbance mode which is directly responsible for spray breakup. Results from the simulations demonstrate theoretical breakup mechanisms which are consistent with experimental observation, and they offer an explanation of an important discrepancy between experiment and the current understanding of pressure-swirl sprays obtained from potential theory.

SUMMARY

The growth of instabilities on the interface between a liquid jet and its gaseous environment is an important mechanism in spray atomization, and it is the subject of the work reported herein. Numerical simulations based on the Navier-Stokes equations were used to model liquid/gas interface flows. An algorithm was developed for solving the unsteady Navier-Stokes equations for incompressible fluid with a discontinuity in density and with surface tension, and its accuracy was demonstrated. In flows representative of round pressure-atomized jets and pressure-swirl atomizers, nonuniform mean velocity distributions resulting from viscous boundary layers were found to have a significant effect on instability growth. In a round jet, the inclusion of a boundary layer-like velocity profile significantly reduced the growth rate of small wavelength instabilities. The velocity profile had a much greater effect than surface tension on the initial atomization process for the flow parameters considered. A good estimate of initial fuel droplet size was obtained by considering boundary layer effects but disregarding surface tension. In a flow representative of the fuel issuing from a pressure-swirl nozzle, nonuniformity of the velocity profile was found to increase the growth rate of a disturbance mode which is directly responsible for spray breakup. Results from the simulations demonstrate theoretical breakup mechanisms which are consistent with experimental observation, and they offer an explanation of an important discrepancy between experiment and the current understanding of pressure-swirl sprays obtained from potential theory.

Keywords: Fluid Dynamics, Computational Fluid dynamics (CFD)

INTRODUCTION AND OBJECTIVES

Liquid fuel for jet and rocket engines must be atomized prior to evaporation and combustion, and the atomization process plays a critical role in determining some combustion properties. For example, large fuel drops cause problems such as fuel deposition on the combustor liner and premature engine failure. Incomplete atomization may occur at low air or fuel flow rates which causes difficulties in starting engines or restarting engines at altitude. Good spray characteristics enhance the stability and compactness of combustion. Two types of atomizers, pressure-swirl atomizers and pre-filming air blast atomizers, are widely used in modern military and commercial gas turbine engines. In both types of devices, a quasi-steady stream of fuel encounters air at a different velocity, and the resulting shear initiates the fuel atomization process.

The mechanisms governing atomization are poorly understood at present. The initial atomization regime involves small spatial and temporal scales, and it is optically dense. Thus, it is difficult to study the physical flows and gain an understanding of atomization. Analysis has been used to study the fundamental fluid mechanisms of simple liquid/gas flows (e.g., Refs. 1,2), and an understanding of some spray behavior has been achieved. However, many observed spray phenomena are not consistent with current theories (Refs. 3,4). Many analyses have employed potential flow models which cannot fully represent the physics of spray atomization. These analyses may give a limited or unrealistic portrayal of atomization mechanisms.

The approach taken in this work was to study atomization by using numerical simulations which accurately represent the fluid physics. Atomization involves incompressible viscous two-phase flow with surface tension; evaporation and combustion can be neglected in the initial atomization region. The Navier-Stokes equations with a suitable surface tension model are believed to describe adequately the behavior of these flows. These equations were solved numerically, and flow phenomena which govern atomization were studied.

Fuel sprays involve complex fluid mechanics and a wide range of time and length scales. In the future it may be possible to simulate many aspects of these complex flows. At present, however, it is possible to simulate only a small range of the atomization process. A substantial body of evidence suggests that the growth of instabilities on the interface between the liquid fuel and the air is a critical part of the initial atomization process (e.g., Refs. 4,5). Hence, the objective of this work was to investigate the growth of instabilities on liquid jets operating in a gaseous environment.

BRIEF CHRONOLOGY OF RESEARCH EFFORT

Initially, it was planned to acquire existing numerical methods and to use them to study instability growth in two phase flows. An evaluation of available methods, including some whose claimed capabilities included the ability to simulate liquid/gas flows, revealed that none had the properties deemed necessary for this work. The methods' ability to conserve exactly quantities such as mass and momentum is vital to the accuracy of simulations

of flows with discontinuities; non-conservative methods are known to represent the propagation of discontinuities with poor accuracy, which would be a serious flaw in the present work. The SOLA-VOF method of Hirt et al (Ref. 6) has been used to simulate multiphase flow, but it employs conservation equations for the velocities, u_i, rather than for the momenta, ρu_i. The "velocity-conservation" equations are equivalent to momentum conservation equations only if the density is constant. The Navier-Stokes algorithm employed by McMurtry et al (Ref. 7) does conserve momentum for constant and variable density flows, but it gives solutions which do not exactly satisfy the incompressibility constraint in variable density flows. This is not likely to be a problem in flows with slow density variations, but it could introduce serious errors in fuel spray flows which have large discontinuities in density. The particle in cell (PIC) method (e.g., Ref. 8) has been used to perform simulations of compressible multiphase flow. However, compressible methods are not well suited for incompressible flow problems, and the high acoustic speed in many fluids would make the flow equations very stiff and, hence, expensive to solve.

It was also discovered that the methods for resolving the density jump and computing the surface tension force at the interface had poor accuracy. The VOF surface tracking method has been observed to give spurious growth of instabilities at an interface (Ref. 6). The SLIC method (Refs. 9,10) may tend to cause the interface to align with the numerical grid (Ref. 11). Either of these types of errors could compromise the accuracy of the simulation method and affect the predicted physical behavior of spray atomization in ways that would be difficult to discern.

Consequently, it was necessary to develop new numerical methods to achieve the objectives of this study. It was difficult to develop a method which is conservative near the sharp density jump at the liquid/gas interface while satisfying the incompressibility constraint; however, it is most critical that the method be conservative at the interface. A numerical algorithm for incompressible variable density flow was developed which satisfies the conservation requirement, the incompressibility constraint, and was sufficiently accurate for the present needs. It is presented in the Research Results section. A computer code which implemented this algorithm was written, and this took a considerable amount of time. Development of the surface tension method was also difficult and time consuming. However, satisfactory solutions to the many numerical problems were found, and an accurate flow prediction code was assembled.

The accuracy of the code was verified for a range of flows for which known solutions existed, including single phase flow in a square cavity, convection of the liquid/gas interface in a uniform flow, and four flows involving growth of liquid/gas instabilities. In all but one of these cases the method gave very good agreement with analytical or other computational results, after suitable grid refinement studies were completed. In the one remaining case, a moderate level of error was attributed to inadequate grid resolution rather than any flaws in the method. Several of the known solutions used for comparison were from potential theory, and it was difficult to reduce the "numerical" diffusion in the Navier-Stokes solutions to low enough levels so that the potential and Navier-Stokes solutions agreed well. Results from two of these cases are presented in the Research Results section. The solutions' dependence on numerical viscosity suggested that the effects of physical viscosity could also be significant, as was later verified.

The growth of instabilities in two flows representative of the initial regions of fuel sprays were studied. One flow was a single liquid/gas interface typical of a pressure-atomized round jet. It is appropriate to study this flow because some fundamental mechanisms are present in both pressure-atomized round jets and in pressure-swirl gas turbine sprays. Also, the simple geometry of round jets is well suited to basic studies of atomization mechanisms, and some data for these sprays exist that can be compared to numerical predictions. For this problem, the simulation method was verified against theo· and experimental data. The other flow was a planar liquid jet which is representative of flow issuing from a pressure-swirl fuel nozzle. The present investigation is one of few which has employed the Navier-Stokes equations as the flow model for a study of atomization. Viscous effects were found to play an important role in the growth of instabilities in both cases, and the study was drawn in that direction.

The significant results from this work can be grouped into two categories. One includes the numerical methods needed to simulate liquid/gas flows; the other concerns the behavior of liquid/gas interface flows and the relevance of this behavior to spray atomization. These are discussed in the Research Results section.

RESEARCH RESULTS

Numerical Methods

Algorithms for solving the incompressible Navier-Stokes equations for variable density fluid and for modeling surface tension effects in a Navier-Stokes calculation were developed in the present work.

The Navier-Stokes method is similar to the commonly used fractional steps algorithm of Chorin (Ref. 12), but modifications to the algorithm and the grid were needed to treat variable density flows. The Navier-Stokes equations apply to the momenta, while the incompressibility condition imposes a constraint on the velocities. The algorithm must compute velocities from the momenta for the so-called corrector part of the algorithm, so that the incompressibility constraint can be satisfied. For this step the density must be known with good accuracy. Methods which use staggered-grid discretization schemes require interpolation of the density, which is very difficult to do accurately at the interface. Hence, the new algorithm uses a cell-centered (i.e., non-staggered) grid, and interpolation is avoided in this step.

A summary of the Navier-Stokes algorithm is given here. The density at the new time level t^{n+1} is computed with the mass conservation equation, and the momentum is estimated with the Navier-Stokes equations in which the pressure terms have been omitted.

$$\frac{\rho^{n+1} - \rho^{n}}{\Delta t} = - \frac{\partial \rho u_i^{n}}{\partial x_i} \qquad (1)$$

$$\frac{\rho u_i^* - \rho u_i^n}{\Delta t} = -\frac{\partial}{\partial x_j}[\rho u_i^n u_j^n + \tau_{ij}^n] + S_i \qquad (2)$$

in which ρ is density, u_i are the velocity components, τ_{ij} is the viscous stress tensor, and S_i is a source term which represents surface tension. The momenta are then corrected to their values at t^{n+1} by

$$\frac{\rho u_i^{n+1} - \rho u_i^*}{\Delta t} = -\frac{\partial p^{n+1}}{\partial x_i} \qquad (3)$$

after the pressure is determined from a Poisson equation. The Poisson equation is obtained by dividing Equation (3) by ρ^{n+1}, taking its divergence, and applying the divergence-free condition $\partial(\rho u_i^{n+1}/\rho^{n+1})/\partial x_i = 0$.

$$\frac{\partial}{\partial x_i}\frac{1}{\rho^{n+1}}\frac{\partial p^{n+1}}{\partial x_i} = \frac{1}{\Delta t}\frac{\partial \rho u_i^*/\rho^{n+1}}{\partial x_i} \qquad (4)$$

If p^{n+1} exactly satisfies Equation (4), then the velocity field at the new time level $u_i^{n+1} = \rho u_i^{n+1}/\rho^{n+1}$ is divergence free. Exact numerical conservation of momentum is ensured by conservation-law discretization of Equations (2) and (3).

The variable density in the Poisson equation causes two minor difficulties. It precludes the use of many fast solvers, and it causes the character of the equation to be nearly hyperbolic at the interface. The Navier-Stokes method is, thus, somewhat expensive to use; however, it is accurate.

The components of the surface tension force may be treated as momentum source terms in the Navier-Stokes equations. The source terms must be consistent with the physics of flows affected by surface tension. Surface tension generates vorticity only at the liquid/gas interface. Also, the surface tension force is exactly balanced by the pressure field at a static interface, such as in a drop at rest. The source terms must be constructed so that both constraints are satisfied. The vorticity constraint is met by computing the surface tension source terms from the gradient of a potential field which has a cut at the interface. This insures that vorticity is generated only at the interface. The exact balance at a static interface is achieved by defining the potential at the same points as the pressure and by employing the same differencing expression to compute the source terms and the pressure gradient terms in the momentum equations.

Other details of the numerical method are discussed by Childs and Mansour (Ref. 13). For the most part, these aspects are not new, but some are critical to the method's accuracy.

The accuracy of the numerical method was demonstrated for several flows for which known solutions exist. The results of two of these are summarized here.

The Rayleigh instability causes a low speed liquid jet to break up due to surface tension. Rayleigh breakup has been studied experimentally, theoretically, and computationally, and it is well understood. The radius of an axisymmetric liquid jet with a single disturbance mode can be described by

$$r = a + \epsilon e^{(ikx + \alpha t)}$$

in which a is the undisturbed radius, x is distance along the jet axis, k is the disturbance wave number, and ϵ is the initial disturbance magnitude. The growth rate of the disturbance α has been determined by potential theory to be

$$\alpha^2 = \frac{\sigma}{\rho a^3} ak\,(1-a^2k^2)\,\frac{I_1(ak)}{I_o(ak)}$$

in which I_o and I_1 are modified Bessel functions of the first kind. The accuracy with which the normalized growth rate $\alpha/(\sigma/\rho a^3)^{1/2}$ is predicted by the simulation is a good test of the method's accuracy, as the growth rate results from a balance between fluid dynamic and surface tension forces. Figure 1 gives the growth rate from theory and from the Navier-Stokes simulation. The predicted growth rates are relatively accurate, but fall below the theoretical result by a few percent. This test demonstrates that the numerical method accurately resolves the relative effects of surface tension and fluid dynamic forces.

A second test of the method's accuracy involves instability growth on a single liquid/gas interface with a high speed liquid and negligible surface tension. This test represents an atomization mechanism which occurs in round and conical jets. Taylor (Ref. 14) studied this flow with potential analysis and determined the normalized growth rate to be

$$\alpha/Uk = R/(1 + iR)$$

in which U is the velocity difference and R is the square root of the ratio of gas to liquid densities. Figure 2 gives the growth rate from theory and predicted by the simulations. Again, the simulations give good accuracy. There is some scatter in the computed results which deserves explanation. Numerical viscosity is present in these calculations which causes the thin shear layer between the high speed liquid and the stagnant gas to grow. The disturbance growth rate decreases as the shear layer becomes thicker. Grids with different grid spacings were used, and the resulting variations in numerical viscosity produced the scatter in the predicted growth rate. The scatter indicates the level of uncertainty which may be expected in other calculations of similar flows using "reasonable" numerical grids.

These tests demonstrated that the numerical method accurately predicts the basic surface tension and fluid dynamic phenomena which affect atomization. Provided that sufficient grid resolution is afforded, simulations based on this method accurately predict the fluid dynamic response of the liquid/gas interface.

Atomization Mechanisms

The growth of initial instabilities on a liquid/gas interface is affected by viscous and inviscid phenomena, surface tension, and the ratio of liquid to gas density. Previous studies have employed potential flow analyses which can address all issues except viscous effects. From these analyses, an "understanding" of some initial atomization mechanisms was formed which is widely held. However, the present work indicates that viscous phenomena have a significant effect on instability growth. Some conclusions drawn from the potential flow analyses may be so altered by viscous effects that they are not applicable in many sprays.

In a pressure-atomized round liquid jet, a viscous boundary layer forms in the nozzle which reduces the fuel velocity at the jet's edge. As the jet exits the nozzle, it is surrounded by a boundary layer of slower fuel. The ratio of boundary layer thickness to instability wavelength δ/λ is one simple measure of viscous effects. Calculations of instability growth rates were done for a range of δ/λ, with the boundary layer in the liquid or in the gas. The flow with the boundary layer in the liquid is representative of flow just exiting the nozzle and is discussed here. The liquid density was taken to be ten times greater than the gas density, and the dependence on density ratio was not investigated. If $\delta/\lambda < 0.1$, the instabilities grow according to potential theory, for which the growth rate increases linearly with the inverse of the wavelength. With increasing δ/λ the growth rate falls significantly below that predicted by potential theory, and for $\delta/\lambda > 0.3$ waves cease to grow. Hence, the presence of a viscous boundary layer suppresses the growth of small wavelength instabilities on pressure-atomized liquid jets, just as surface tension does. Long wavelength disturbances grow slowly in accordance with potential theory, and short ones grow slowly or not at all, because of viscous effects. The maximum growth rate occurs at some intermediate wavelength. The characteristics of this most amplified wave can be used to estimate spray properties such as initial drop size and spray angle.

Estimates of drop sizes were made for the sprays which Wu et al (Ref. 3) studied experimentally. The drop sizes estimated from the most amplified wave in a flow which had a boundary layer were roughly 250% of the measured values. A potential flow analysis which included surface tension but not the boundary layer effects gave a drop size estimate which was roughly 5% of the measured value. This result indicates that the boundary layer mechanism is significantly more important than the surface tension effects in controlling the initial atomization process in pressure-atomized sprays, for the operating parameters used in these sprays. This result also has an important implication for modeling of spray systems. While the potential flow results suggest that droplet coalescence must occur to achieve the measured drop size, the present results suggest that droplet breakup may be occurring.

The growth of instabilities which affect atomization of the flow from pressure-swirl nozzles have also been studied. The fuel flows from a pressure-swirl nozzle as a diverging annular jet which may break into ligaments and then into drops. There are believed to be two dominant instabilities which grow on the jet, the "antisymmetric" mode which causes the jet to become sinuous but not to break up, and the "symmetric" mode which causes the jet to break into ligaments. Potential flow analyses predict that

the antisymmetric mode grows much more rapidly than the symmetric mode for all flow conditions. In accordance with this theory, the antisymmetric mode is often observed in pressure-swirl sprays, such as that shown in Figure 3(a). However, rapid breakup occurs in some sprays in a manner which suggests that the symmetric mode can grow more rapidly than the antisymmetric mode, as shown in Figure 3(b). The theoretical understanding of atomization from potential flow analysis cannot explain the spray behavior displayed in Figure 3(b). This discrepancy between theory and experiment reflects the poor understanding of the fundamental mechanisms which govern atomization in pressure-swirl sprays.

The fuel flow in the nozzle has a complex three-dimensional boundary layer at the nozzle wall which causes nonuniformity in the fuel jet. The growth of instabilities on the jet may be affected significantly by the nonuniformity. A model problem which represents some essential aspects of flow from pressure atomizers is a planar liquid jet. An appropriate velocity field for the jet was not known, and it was therefore approximated with a simple quasi-linear velocity profile with zero velocity on one edge of the jet and a maximum near the other edge. This flow was studied to assess the importance of viscous effects on pressure atomizers. Compared to a uniform velocity profile, the quasi-linear profile increases the growth rate of the symmetric mode significantly, but has a small effect on the antisymmetric mode, as shown in Figure 4. The symmetric mode grows more rapidly than the antisymmetric mode for small values of the ratio of the disturbance's wavelength to the liquid jet thickness. In the spray from a pressure-swirl nozzle, more rapid growth of the symmetric mode would cause the fuel jet to break up into ligaments and then into drops without sinuous distortions of the jet. This may be the mechanism which causes the rapid breakup shown in Figure 3(b).

With results from the present simulations and potential theory, a possible explanation of the two types of spray breakup in Figure 3 can be proposed. If the liquid jet is at a low Reynolds number, viscous effects will cause the velocity profile in the jet to become uniform shortly after it leaves the nozzle and before inertial forces can cause it to break up. In this case, the antisymmetric disturbance mode will dominate the breakup process as predicted by potential theory, and a sinuous conical jet similar to Figure 3(a) will result. In a high Reynolds number liquid jet, the viscous forces do not cause the velocity profile to become uniform before inertial forces cause the jet to break up. In this case, the symmetric disturbance mode can dominate the spray breakup, and the type of spray behavior shown in Figure 3(b) would occur. Thus, the large growth rate of the symmetric mode observed in the simulations may explain the rapid jet breakup observed in some pressure-swirl sprays.

SUMMARY OF ACCOMPLISHMENTS

Fundamental Atomization Mechanisms

- Viscous boundary layers were demonstrated to have a large effect on the growth rates of instabilities which contribute to atomization.

- Surface tension was shown to be less important than boundary layer effects in the initial atomization process of some pressure-atomized round liquid jets.

- The droplet size in the initial atomization region of a fuel jet issuing from a circular nozzle was estimated with good accuracy.

- On a planar liquid jet which is representative of flow issuing from a pressure-swirl atomizer, it was shown that the growth rate of an instability which leads directly to jet breakup is increased by nonuniformity of the jet's velocity profile. This basic flow phenomenon may be the mechanism which causes rapid atomization in some pressure-swirl sprays.

Numerical Algorithms

- An algorithm for solving the Navier-Stokes equations for a variable density incompressible flow was developed.

- The requirements for modeling surface tension numerically were delineated, and accurate calculations of surface tension phenomena were demonstrated.

RECOMMENDED FUTURE RESEARCH

The use of numerical simulations to study atomization is in its infancy, and the potential of this approach is difficult to assess. It offers the possibility of understanding fundamental processes which are very difficult to probe experimentally. In the present work, relatively simple but accurate methods were used to explore the physics of a rather limited class of flows. Important new insights into the atomization mechanisms of round jets and pressure-swirl sprays were obtained. To explore a wider range of atomization phenomena, more advanced numerical methods may be required.

Future work is needed to develop methods which can treat the complex liquid/gas interface that occurs when, for example, drops break up or coalesce. Existing methods have poor accuracy and, in practice, appear to suffer from some serious flaws. Distortions of the interface which appear to be caused by numerical errors rather than modeled physics have been observed in calculations with several methods. Further work on methods for modeling surface tension is also appropriate.

There are aspects of atomizer flows for which improved understanding can be achieved and, perhaps, translated into improved performance. Large drops from pressure-swirl nozzles are caused, in part, by streaks on the conical

fuel jet and, presumably, by flow nonuniformity or interface waves on the air core within the nozzle. The importance of the flow within pressure atomizers has been emphasized by many researchers. This flow can be simulated computationally to investigate possible sources of the streaks and to study means of suppressing the streaks. The atomization process depends on the mean velocity profile, and this dependence could be mapped. It might then be possible to determine nozzle exit velocity profiles which give acceptable atomization under difficult operating conditions. Thus, it may be possible to exert control over the atomization process in a pressure-swirl spray.

PUBLICATIONS

The results of this work are described in the paper entitled "Simulation of Fundamental Atomization Mechanisms in Fuel Sprays," AIAA-88-0238, co-authored by N. N. Mansour. It was presented at the AIAA 26th Aerospace Sciences Meeting, Reno, Nevada. This paper has been submitted for publication in the AIAA Journal of Propulsion and Power.

TECHNICAL PERSONNEL

Dr. Robert E. Childs and Dr. Nagi N. Mansour worked on this project.

NEW DISCOVERIES

The new discoveries are described in the "Research Results" section of this report. There were no inventions or patent disclosures resulting from this work.

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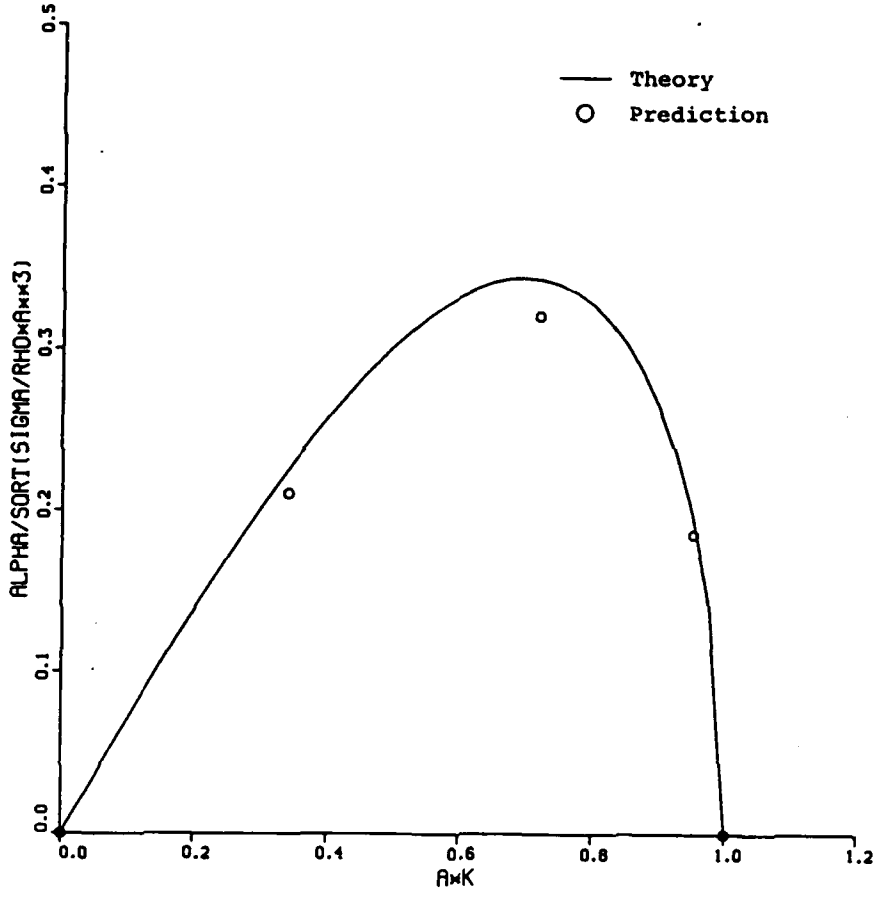


Figure 1. Comparison of potential theory and present numerical predictions for growth rate of Rayleigh instability of round liquid jet as a function of wave number.

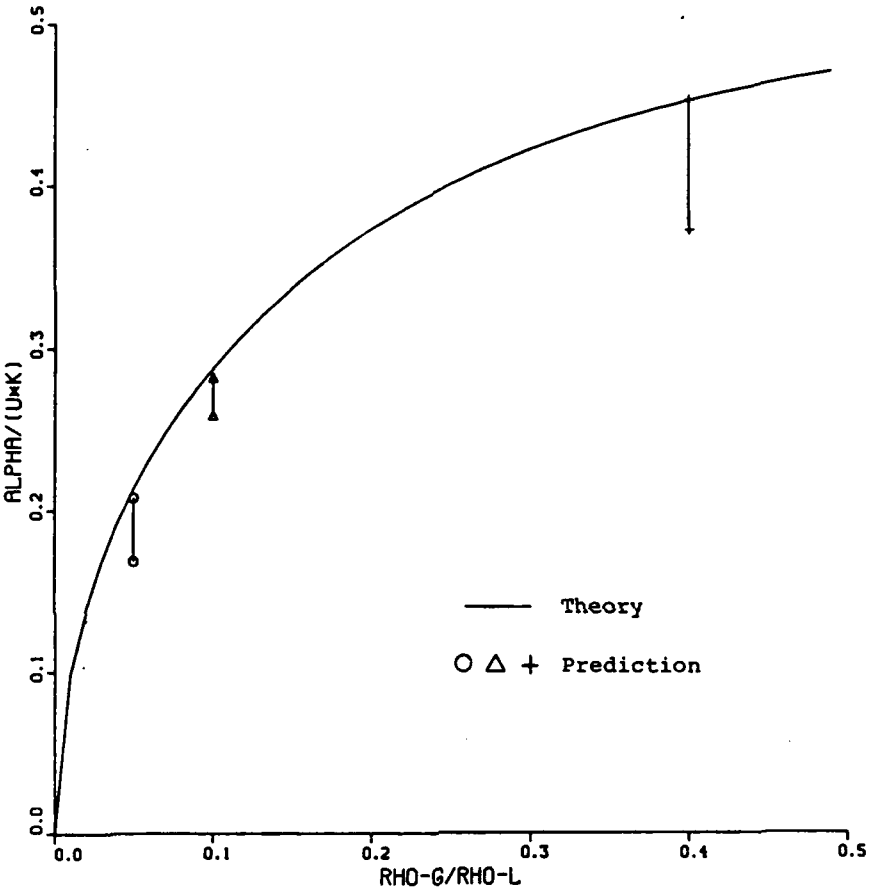
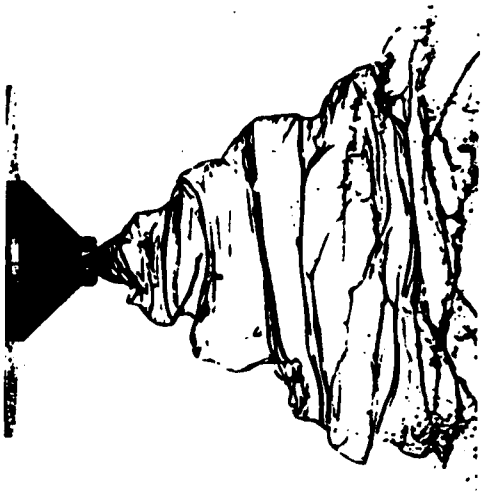
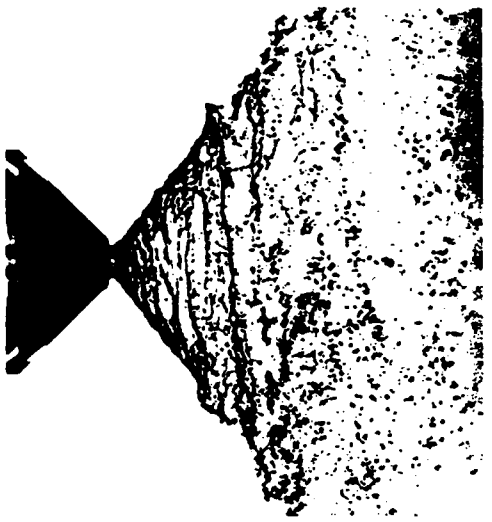


Figure 2. Comparison of potential theory and present numerical predictions for growth rate of wind induced-instability on a single planar interface as a function of gas to liquid density ratio.



(a) Breakup dominated by "antisymmetric" mode.



(b) Breakup dominated by "symmetric" mode.

Figure 3. Different modes of atomization in pressure-swirl sprays. (Photographs by Eugen Klein, from Van Dyke, Ref. 15)

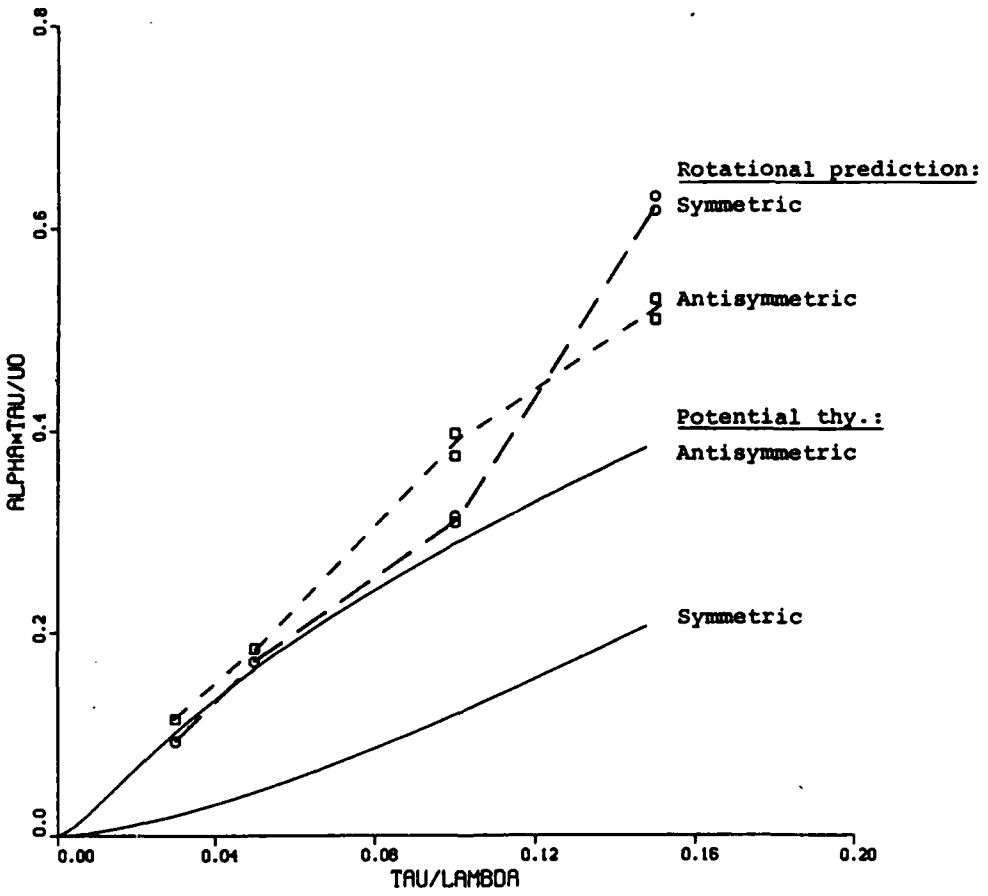


Figure 4. The growth rate of the symmetric and antisymmetric modes on a planar liquid jet as a function of the ratio of jet thickness to disturbance wavelength. Results from potential theory and from simulations involving a jet with a non-uniform (rotational) velocity profile.