NUMERICAL SIMULATION OF LIQUID-GAS INTERFACES WITH APPLICATIONS TO ATOMIZATION

Thomas Boeck, Stéphane Zaleski
Laboratoire de Modélisation en Mécanique
4 place Jussieu, 75005 Paris
Email: zaleski@lmm.jussieu.fr

Summary
We investigate the two-phase mixing layer between high speed liquid and gas jets. This flow leads to the breakup of the interface into small droplets and is the basic mechanism in atomization processes. We use Volume of Fluid methods to investigate this flow numerically. Some recent versions of the Volume of Fluid method conserve momentum exactly, which is an advantage for the robust simulation of very small droplets. To validate the use of these methods for the computation of the instability, we have investigated in depth the linear stability theory. Good agreement is obtained between simulations and stability theory. We then report simulations of the non-linear development of the instability in 3D. We use boundary conditions that allow the study of the spatial development of the instability. The simulations show the convective character of the instability and the influence of small upstream perturbations on droplet formation.

INTRODUCTION: THE ATOMIZATION PROBLEM

Atomization phenomena are important in combustion engines as well as in many other processes. Several mechanisms lead to atomisation, such as upstream turbulence, cavitation and the Kelvin-Helmholtz instability in the sheared liquid-gas interface [1, 2, 3]. The development of this instability leads to very complex structures, the study of which is the focus of this lecture. Numerical simulation of these flows is a major challenge for large scale computational fluid dynamics. The LMM group has developped a number of interface tracking methods, among which Volume of Fluid is particularly of interest. Some versions of the Volume of Fluid methods conserve momentum exactly [4], which is an advantage for the simulation of small droplets. However fundamental difficulties remain with the use of these methods. One is that it is very difficult to simulate flows which are simultaneously at (i) large Reynolds number Re (ii) large Weber number We (iii) large values of the density ratio ρ_l/ρ_g and (iv) large values of the viscosity ratio μ_l/μ_g. While it is possible to tune the codes so that large values of all the numbers are reached, doubts may reasonably remain on the accuracy of the result. Thus it is very important to find validation cases. The comparison between linear theory and predictions of the numerical simulations is particularly of interest here. Very few such validations exist with the exception of the work of Tauber, Unverdi and Tryggvason [5]. Moreover, the in-depth investigation of linear theory is interesting in its own right as it sheds light on the mechanisms of the Kelvin-Helmholtz instability.

LINEAR STABILITY THEORY

The simplest version of linear instability theory assumes a staircase-like velocity profile and the temporal development of the instability. Viscosity is neglected. This version predicts a critical Weber number above which instability develops [6].
A more realistic theory is obtained assuming a piecewise-linear velocity profile. These profiles represent schematically the boundary layers in the gas and in the liquid. The gas boundary layer forms in the upstream flow inside the nozzle. After the nozzle exit, both boundary layers evolve under the action of viscosity [7, 8]. The piecewise linear profiles were employed in the theoretical work of E. Villermaux and coworkers. The experimental and theoretical power laws agree but the prefactors do not for axially symmetric flow [9], a result still not understood. It is interesting to note that until now quantitative agreement was very difficult to find between linear theory and numerical simulations as well.
Recently a much more realistic linear theory of atomization was developed by Phil Yecko and one of the authors [10, 11]. It uses smoothly varying boundary layer profiles and solves the full linearized viscous equations, i.e. the Orr-Sommerfeld equations. The error function profiles have advantages in the comparison with numerical simulation as they are slowly varying in time at small viscosity. Excellent agreement is then obtained with the full numerical simulation for relatively small values of the viscosity ratio. There is a large difference with the inviscid theory (Fig. 1a).
An interesting feature of the Orr-Sommerfeld theory is that one obtains, for sufficiently large Reynolds numbers, several new instability modes [10, 11]. These modes are in some sense similar to Tollmien-Schlichting modes: some of them tend to disappear albeit slowly for large Reynolds numbers, while one of them remains and converges very slowly to the inviscid modes. Some of the modes are clearly related to viscous effects and seem for large We to be a continuation of the "Hinch modes" [12].

NUMERICAL METHODS

To solve the fully nonlinear problem, we use a version of the Volume of Fluid method. The method has been thoroughly described in several recent references [13, 4, 14]. In short, we use a volume fraction C_{ij} to describe the fraction of liquid filling a cell ij. The interface is reconstructed and advected at each time step. The Navier-Stokes equations with variable

viscosity and surface tension are solved for an incompressible fluid using a finite volume method on a square lattice. Surface tension is treated by a "Continuous Surface Force" method, smoothing the surface tension term in the equations over two or three grid cells. The incompressibility constraint is obtained using a projection method, with a multigrid algorithm for the pressure. Details will be given in the full lecture. Agreement with linear theory is excellent when the viscosity ratio is small. When the viscosity ratio is large, however, one needs to pay attention to the viscosity in mixed cells. The correct exponential behavior is obtained for a mixed-cell viscosity given by the harmonic mean

$$\mu_{ij} = [\mu_l^{-1} C_{ij} + \mu_g^{-1}(1 - C_{ij})]^{-1} \tag{1}$$

This expression for the mixed cell viscosity had already been proposed by Patankar and used in [15], however it is here shown for the first time to have a large effect on the linear growth regime.

NONLINEAR DEVELOPMENT OF THE INSTABILITY

The nonlinear stages of the instability show the development of 2D sheets, followed by the growth of 3D filaments or fingers. An example of the temporal development is shown in Figure 1a. We also use entry and exit conditions and study the spatial development of the instability. Small perturbations are imposed near the flow entrance. These pertubations create velocity fluctuations of the order of 10 % of the mean flow. When these perturbations are present the instability develops in a manner similar to the experimental observations. In the absence of perturbations the nonlinear development does not occur. This is interpreted as an effect of the convective character of the instability. We measure the size of the detached droplets at various times in the simulation. The observed distribution of droplet sizes is exponential as observed in the experiments.

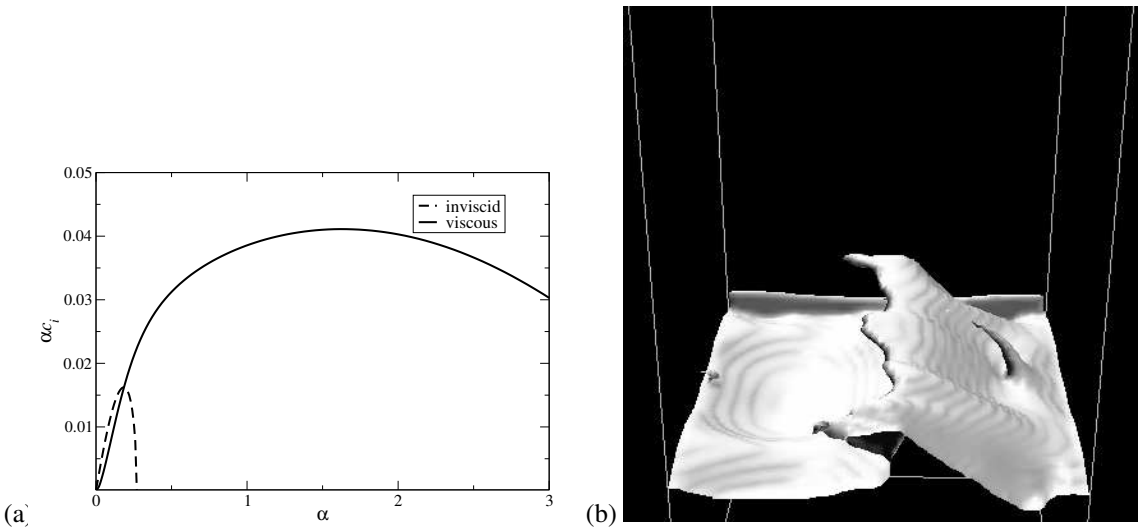

Figure 1. (a) Comparison of inviscid and viscous results, the parameters are $We_g = 200, Re_g = 1000, \mu_g/\mu_l = 0.025, \rho_g/\rho_l = 0.02$ (b) 3D temporal growth of the instability. $\rho_g/\rho_l = 0.1, We_g = 200, Re_g = 1000$, the grid size is 128^3.

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