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NUMERICAL METHOD FOR TWO-PHASE FLOW DISCONTINUITY PROPAGATION CALCULATION

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ABSTRACT

In this paper, we present a class of numerical shock-capturing schemes for hyperbolic systems of conservation laws modelling two-phase flow. First, we solve the Riemann problem for a two-phase flow with unequal velocities. Then, we construct two approximate Riemann solvers: a one intermediate-state Riemann solver and a generalized Roe's approximate Riemann solver.

We give some numerical results for one-dimensional shock-tube problems and for a standard two-phase flow heat addition problem involving two-phase flow instabilities.

INTRODUCTION

Computation of complex two-phase flows is required to simulate a wide variety of industrial systems behavior under normal or accidental conditions. For the modelling of two-phase flow, several sets of equations ranging in complexity from a simple homogeneous equilibrium model to a very complicated two-fluid model involving unequal pressure for each phase, have been worked out. This paper is devoted to the well-known Drift-Flux model which has been widely used for the analysis of thermal-hydraulics transients.

Most of numerical methods used in two-phase flow computer codes like TRAC¹, SIMMER², are based upon semi-implicit finite difference schemes with staggered grids and upwind differencing. The main features of these schemes are their efficiency and their robustness, but they are not suitable for flow problems requiring resolution of shock or discontinuity propagation. This is due to numerical diffusion introduced by donor-cell differencing and by the reduction to an elliptic problem of the pressure propagation.

In this paper, we present a new class of numerical shock-capturing schemes for hyperbolic system of conservation laws modelling two-phase flow, based on nonlinear approximations. Such numerical schemes have been first developed for nonlinear scalar equations and have been

formally extended to nonlinear hyperbolic systems of conservation laws through the use of exact or approximate Riemann Solvers³⁻⁵. It is emphasized that these Riemann solvers, as originally developed, are only valid for a perfect gas (and a single phase).

The objective of this paper is to show that this Riemann solver approach can apply to hyperbolic two-phase flow models. We begin by the study of the Riemann problem for the Drift-Flux model. Then, we construct approximate Riemann solvers and describe the corresponding Godunov type schemes as well as two dimensional extensions.

THE DRIFT-FLUX MODEL

The Drift-Flux model for a two-phase flow as mixture of liquid and vapor, consist of two phasic mass conservation equations, one mixture momentum conservation equation and one mixture energy equation. This leads to a system of four partial differential equations:

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(\alpha \rho_v) + \frac{\partial}{\partial x}(\alpha \rho_v u_v) = \Gamma \\ \frac{\partial}{\partial t}((1-\alpha)\rho_l) + \frac{\partial}{\partial x}((1-\alpha)\rho_l u_l) = -\Gamma \\ \frac{\partial}{\partial t}(\alpha \rho_v u_v + (1-\alpha)\rho_l u_l) + \frac{\partial}{\partial x}(\alpha \rho_v u_v^2 + (1-\alpha)\rho_l u_l^2 + p) = -\tau - (\alpha \rho_v + (1-\alpha)\rho_l)g \\ \frac{\partial}{\partial t}(\alpha \rho_v (h_v + \frac{u_v^2}{2}) + (1-\alpha)\rho_l (h_l + \frac{u_l^2}{2}) - p) + \frac{\partial}{\partial x}(\alpha \rho_v u_v (h_v + \frac{u_v^2}{2}) + (1-\alpha)\rho_l u_l (h_l + \frac{u_l^2}{2})) = q + f_b \end{array} \right. \quad (1)$$

In the system (1) the v and l subscripts refer to vapor and liquid phases respectively. The variables appearing in the above system have the following meanings: α is the volume void fraction, $\rho_{v,l}$ is the phasic density, $u_{v,l}$ is the phasic velocity, $h_{v,l}$ is the phasic specific enthalpy and p is the common pressure. In the right-hand side, Γ is the interphase mass exchange, g is the gravity constant, τ represents the wall friction, q is a heat source and f_b represents some body forces.

To close the system we need additional relationships which are given by constitutive equations. We assume that state equations giving the phasic density as a function of the phasic specific enthalpy and pressure are available:

$$\rho_v = \rho_v(p, h_v) \quad \text{and} \quad \rho_l = \rho_l(p, h_l).$$

A relative velocity correlation is expressed, according to the Drift-Flux model, in the following form:

$$\Delta u \equiv u_v - u_l = (1-\alpha)^{k-1} v_{\infty} \quad (2)$$

The index k , fitted by experiment, is positive and v_{∞} is a constant velocity of rising bubbles in an infinite medium.

Since the model presented above provide only a single energy equation, an additional thermal constraint is necessary. A variety of such constraints is possible, the simplest of which is the assumption of thermal equilibrium between phases.

THE RIEMANN PROBLEM FOR TWO-PHASE FLOW

In our discussion, we do not take into account the heat source, viscosity or friction effects and concentrate our attention on the non linear transport effects. For this purpose, we study the Riemann problem which is a particular Cauchy problem for (1) corresponding to a discontinuous initial data:

$$U(x,0) = U_L \quad \text{if } x < 0, \quad U_R \quad \text{if } x > 0, \quad (3)$$

where U_L and U_R are two given constant states. Moreover, for the construction of numerical schemes based upon Riemann solvers, it will be sufficient to consider the following (simplified) system without the energy conservation equation:

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} f(U) = 0 \quad (4)$$

with

$$U = \begin{bmatrix} \alpha \rho_v \\ (1-\alpha)\rho_l \\ \alpha \rho_v u_v + (1-\alpha)\rho_l u_l \end{bmatrix} \quad \text{and} \quad f(U) = \begin{bmatrix} \alpha \rho_v u_v \\ (1-\alpha)\rho_l u_l \\ \alpha \rho_v u_v^2 + (1-\alpha)\rho_l u_l^2 + p \end{bmatrix}$$

In the Drift-Flux model attention is focused on the relative motion Δu rather than on the velocity of the individual phases. In the simplest case where $\Delta u \equiv 0$, the system (4) reduces to the homogeneous system which is very similar to the Euler equations. Otherwise, in many physical interesting situations, we may assume that the relative velocity Δu is small compared to the mixture sound speed c_m given by

$$\frac{1}{c_m^2} = \left[\frac{\partial p}{\partial p} \right]_s = \rho \left(\frac{1-\alpha}{\rho_l c_l^2} + \frac{\alpha}{\rho_v c_v^2} \right)$$

where c_v^2 and c_l^2 denote sound velocity in vapor and liquid phase, respectively. In consequence, we may consider the system (4) as a perturbation of the homogeneous case. Following these remarks, we will first solve the Riemann problem for a flow with equal velocities. Then, the case of a two-phase flow with unequal velocities will be studied by using Taylor expansions according to the variable $\xi = \frac{v_{\infty}}{c_m}$. (in fact, we will limit to first order approximation; straightforward computations gives higher order approximations.)

EQUAL VELOCITIES

In that case $v_{\infty} \equiv 0$ and the system (4) reduces to:

$$\begin{cases} \frac{\partial}{\partial t}(\alpha \rho_v) + \frac{\partial}{\partial x}(\alpha \rho_v u) = 0 \\ \frac{\partial}{\partial t}((1-\alpha)\rho_l) + \frac{\partial}{\partial x}((1-\alpha)\rho_l u) = 0 \\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = 0 \end{cases} \quad (5)$$

where u is the common velocity and $\rho = \alpha\rho_v + (1-\alpha)\rho_l$ is the mixture density. The eigenvalues of (5) are given by:

$$\lambda_1 = u - c_m, \quad \lambda_2 = u, \quad \lambda_3 = u + c_m.$$

The system (5) is strictly hyperbolic and possesses two genuinely non linear characteristic fields and one linearly degenerate field associated to the eigenvalue λ_2 .

Given a constant state $U_0 = (\alpha_0, p_0, u_0)$, let us define the following wave curves:

$$W^1(U_0) = \left\{ U = (\alpha, p, u) / \alpha = \alpha^0(p) \text{ and } u = \begin{cases} u_0 - \int_{p_0}^p \frac{ds}{\rho c_m(s)} & \text{for } p \leq p_0 \\ u_0 - (\rho - \rho_0) \left[\frac{1}{\rho\rho_0} \frac{p - p_0}{\rho - \rho_0} \right]^{\frac{1}{2}} & \text{for } p \geq p_0 \end{cases} \right\}$$

$$W^3(U_0) = \left\{ U = (\alpha, p, u) / \alpha = \alpha^0(p) \text{ and } u = \begin{cases} u_0 + \int_{p_0}^p \frac{ds}{\rho c_m(s)} & \text{for } p \leq p_0 \\ u_0 + (\rho - \rho_0) \left[\frac{1}{\rho\rho_0} \frac{p - p_0}{\rho - \rho_0} \right]^{\frac{1}{2}} & \text{for } p \geq p_0 \end{cases} \right\}$$

where we set

$$\alpha^0(p) = \frac{\alpha_0 \rho_v^0 \rho_l(p)}{\alpha_0 \rho_v^0 \rho_l(p) + (1 - \alpha_0) \rho_l^0 \rho_v(p)}$$

Proposition: Given two states U_L and U_R , the solution to the Riemann problem (5)-(3) is composed by a 1-wave and a 3-wave which are separated by a contact discontinuity over the void fraction α . The intermediate states are given by the intersection of $W^1(U_L)$ and $W^3(U_R)$.

We refer the reader to Reference 6 for more details.

UNEQUAL VELOCITIES

The velocity u denotes now the volume average velocity, $u = \alpha u_v + (1-\alpha)u_l$. Under the condition $v_\infty \ll c_m$, the eigenvalues of the system (4) remain real velocities and can be computed by using Taylor expansions. For example, the eigenvalue λ_2 is given by

$$\lambda_2 = u + (1-\alpha-k-\alpha)(1-\alpha)^{k-1} v_\infty + v_\infty O(\xi^2).$$

An easy computation gives

$$\nabla_{\lambda_2} r_2 = \frac{\partial \lambda_2}{\partial \alpha} = -k(1-\alpha)^{k-2} (2-(k+1)\alpha) v_\infty + v_\infty O(\xi^2)$$

We remark that $\nabla \lambda_2 r_2$ doesn't keep a constant sign. Thus, limited to first order approximation, we have the following two cases:

- for $0 < k \leq 1$ the 2-characteristic field is genuinely non linear
- for $k > 1$ the 2-characteristic field is neither genuinely non linear nor linearly degenerate

Nevertheless, the other characteristics fields remains genuinely non linear for sufficiently small ξ . To solve the Riemann problem we need, as previously, to describe the wave curves of the system. $W^1(U_0)$ and $W^3(U_0)$ are composed by simple waves (shock or rarefaction) but a complex 2-wave appears. Detailed description of $W^1(U_0)$ and $W^3(U_0)$ can be found in the expanded version of this paper¹⁰. The following proposition describe the 2-wave curve.

Proposition: Let $U(\alpha_0)$ and $U(\alpha)$ be the left and right states on both sides of a discontinuity and Δu be the relative velocity given by (2).

if $k < 1$ then

- Pressure and volumetric velocity are constant, along a 2-wave curve (shock or rarefaction), with a first order approximation according to ξ
- $U(\alpha_0)$ and $U(\alpha)$ are linked by an admissible 2-shock wave if $\alpha > \alpha_0$ or a rarefaction wave in the other case.

if $k \geq 1$ then ; let be I the interval with α and α_0 as extremities and α^* the void fraction value as $\sigma_2(\alpha^*, \alpha_0) = \lambda_2(\alpha^*)$ is the 2-shock wave velocity.

- If $\alpha \in I$, the 2-wave is a single wave : shock wave if $\alpha > \alpha_0$ or a rarefaction wave in the other case.
- If $\alpha^* \in I$, the 2-wave is a double wave which is made of a shock wave $U(\alpha_0)/U(\alpha^*)$ and a rarefaction wave $U(\alpha_0)/U(\alpha^*)$.

GODUNOV TYPE SCHEMES FOR TWO-PHASE FLOW

The resolution of the Riemann problem for two-phase flow requires important analytical efforts but it leads to suitable numerical scheme for computing flows with a very complicated shock structure.

Godunov had used the exact solution of local Riemann problems to obtain an upstream-differencing scheme. This scheme requires an iterative procedure to compute the intermediate states, which leads to time-consuming numerical codes. To overcome this drawback, Harten, Lax and Van Leer³ define a class of approximate Riemann solvers which can have a much simpler structure as long as they satisfy the essential properties of consistency with the conservation equations and the entropy inequality. Then, they define the Godunov-type schemes by replacing the exact solution $U_a(\frac{x}{t}, U_L, U_R)$ to the Riemann problem, by an approximate Riemann solver $U_a(\frac{x}{t}, U_L, U_R)$ in the original Godunov's scheme.

These numerical schemes can be written in conservative form and are of first-order. There exists many ways to achieve second-order spatial accuracy and have at the same time Total Variation Diminishing property. (for example using flux limiters or a predictor-corrector scheme)

Let us now, describe two approximate solvers to the Riemann problem (3)-(4), for the Drift-Flux model.

ONE INTERMEDIATE-STATE RIEMANN SOLVER

Denote by a_L , a_R lower and upper bounds, respectively, for the smallest and largest signal velocity. Harten, Lax and Van Leer⁸ define the following approximate Riemann solver:

$$U_a\left(\frac{x}{t}, U_L, U_R\right) = \begin{cases} U_L & \text{if } \frac{x}{t} \leq a_L \\ U_{LR} & \text{if } \frac{x}{t} \in]a_L, a_R[\\ U_R & \text{if } \frac{x}{t} \geq a_R \end{cases}$$

The intermediate state U_{LR} is chosen to satisfy the conservation laws.

There is no general algorithm for calculating the bounds a_L and a_R for arbitrary initial data (3) but proper estimates may be obtained by an analysis of the exact solution to the Riemann problem. We present in reference 7 an algorithm that calculates the velocities a_L and a_R for the Drift-Flux model. This algorithm provides, with few computational efforts, an attractive scheme on which we can construct higher order extensions.

Since $U_a(\frac{x}{t}, U_L, U_R)$ contains only one intermediate state, the corresponding Godunov-type scheme spreads the 2-wave, and it is a rather rough approximation to the exact solution. To get more accurate approximation, we turn now to describing an approximate Riemann solver based on a Roe's type linearization.

GENERALIZED ROE'S APPROXIMATE RIEMANN SOLVER

Roe¹⁰ considers approximate solution to (3),(4) which are exact solution to the linear approximate problem:

$$\frac{\partial U}{\partial t} + A(U_L, U_R) \frac{\partial U}{\partial x} = 0$$

where the initial data (3) is unaltered and $A(U_L, U_R)$ is a constant matrix satisfying the following Roe's properties

$$A(U, U) = \frac{\partial f(U)}{\partial U}$$

$$f(U_L) - f(U_R) = A(U_L, U_R) \cdot (U_L - U_R)$$

Roe obtained such average matrix for the Euler equations with an ideal equation of state by introducing a parameter vector. Vinokur showed that Roe's construction can be generalized to an arbitrary gas. In reference 11, we construct for the Drift-Flux model, an average matrix $A(U_L, U_R)$ satisfying Roe's properties. Introducing the parameter vector

$$\sqrt{\rho} \left(1, c, u, h + \frac{u^2}{2} \right)$$

where c denotes the concentration, we show that we can draw a parallel with Roe's construction. Our construction involves the mixture density derivatives

$$\mu_1 = \left[\frac{\partial \rho}{\partial p} \right]_h \quad \text{and} \quad \mu_2 = \left[\frac{\partial \rho}{\partial h} \right]_p \quad (5)$$

and also the relative velocity derivatives. The only difficult point is to find approximations $\bar{\mu}_1$ and $\bar{\mu}_2$ to μ_1 and μ_2 satisfying the relation

$$\Delta \rho = \bar{\mu}_1 \Delta h + \bar{\mu}_2 \Delta p \quad (6)$$

Where $\Delta(\cdot) = (\cdot)_L - (\cdot)_R$. It is quite important to note that the eigenvalues of $A(U_L, U_R)$ are strongly dependent of $\bar{\mu}_1$ and $\bar{\mu}_2$ since the speed of sound in the mixture is given by

$$\frac{1}{c_m^2} = \frac{1}{\rho} \mu_1 + \mu_2$$

Thus, these thermodynamics derivatives will have a large effect on the accuracy and the general behavior of the approximate Riemann solver.

When the density derivatives μ_1 and μ_2 are smooth functions of $V = (p, h)$, unique values of $\bar{\mu}_1$ and $\bar{\mu}_2$ satisfying (6) may be obtained by fitting the analytical expressions of μ_1 and μ_2 . However, in two-phase flows as mixture of water and steam, we have to deal with additional difficulties because of the density derivatives discontinuity across the saturation curve.

Let $V_L = (p_L, h_L)$ and $V_R = (p_R, h_R)$ be two states on each side of a given state V^{sat} which belongs to the saturation curve. We remark then, that the relation (6) has no more sense when V_L and V_R tend to the state V^{sat} , since μ_1 and μ_2 are discontinuous at this point. We need more information on how the phase change occurs to compute the approximate derivatives $\bar{\mu}_1, \bar{\mu}_2$. For this purpose, we propose to weaken the relation (6) by setting

$$\Delta \rho = \int_0^1 \frac{\partial \rho}{\partial V}(\Phi(s, V_L, V_R)) \frac{\partial \Phi}{\partial s}(s, V_L, V_R) ds \quad (7)$$

where $\Phi(s, V_L, V_R)$ is a smooth path connecting the two states V_L and V_R :

$$\Phi(0, V_L, V_R) = V_L \quad \text{and} \quad \Phi(1, V_L, V_R) = V_R$$

The main motivation of the relation (7) is that the right-hand side is well defined across the saturation curve. Moreover, the additional informations needed to describe the phase change (for instance vaporization or condensation) can be incorporated into the relation (7) with the help of the family of paths Φ .

For further developements and the complete description of this approximate Riemann solver we refer to Reference 11. Let us only give examples of such family of paths Φ needed to define the approximate derivatives $\bar{\mu}_1$ and $\bar{\mu}_2$.

If V_L and V_R are in the same phase we can take for Φ the straight line connecting V_L and V_R :

$$\Phi(s, V_L, V_R) = V_L + s (V_L - V_R) \quad \text{for } s \in [0, 1]$$

An easy computation yields

$$\bar{\mu}_1 = \int_0^1 \mu_1(V_L + s(V_L - V_R)) ds \quad \text{and} \quad \bar{\mu}_2 = \int_0^1 \mu_2(V_L + s(V_L - V_R)) ds$$

If V_L and V_R are not in the same phase, for example V_L is in a liquid region and V_R is in a two-phase region, we take a path composed of three pieces: the first connects the state $V_L = (p_L, h_L)$ to the state $V_R^{sat} = (p_R, h^{sat}(p_R))$ on the saturation curve, the second follows close on the saturation curve from V_R^{sat} to $V_L^{sat} = (p_L, h^{sat}(p_L))$ and the last links V_L^{sat} to the state V_R . Such paths have been used successfully in the numerical experiments.

TWO DIMENSIONAL EXTENSIONS

For two-dimensional flows, the developed scheme is based upon an approximate Riemann solver with one intermediate state, according to the following principles:

- Since signal velocities are bounded, waves coming from orthogonal directions do not interact outside of a bounded domain dependent of the time step and the signal velocities. In case where orthogonal waves do not interact, fluxes are computed with an approximate one dimensional Riemann solver.
- In the other case, the region where orthogonal waves interact is approximated by a single state calculated from conservation equations deduced relationships.

NUMERICAL RESULTS

The schemes presented here have been tested on both, one-dimensional shock-tube problems (i.e. discontinuous initial data problem) for which analytical solutions are known, and several one and two-dimensional standard problems of practical interest. (phase separation, heat addition, level tracking,...)

Because of space limitation, only two examples of shock-tube problem involving, respectively, a simple and a double 2-wave, and two-phase flow instabilities calculations are presented here.

The figures 1-2 provide a comparison of the Godunov-type scheme with one intermediate-state and the first order Roe's approximate solver. The two schemes give almost the same results except on the 2-wave where the Godunov's scheme is more diffusive.

The figure 3 compares these two schemes on a Riemann problem involving a double 2-wave. The 2-wave's structure is not reproduced by the Godunov's scheme since the corresponding approximate solver contains only one intermediate-state. On the other hand the generalized Roe's scheme yields a sharper capture of void fraction discontinuities.

- The results presented in figures 4-5 concern the prediction of the transient resulting from heat addition to upward liquid flow in a smooth vertical pipe¹³.

CONCLUDING REMARKS

In conclusion, the present study shows the applicability of the Riemann solver approach for hyperbolic two-phase flow models. The numerical results obtained for standard test problems

show that the Godunov-type schemes presented here, give good results for a wide range of flow conditions. These schemes produce accurate solutions near the discontinuities and provide a robust procedure for the treatment of physically relevant boundary conditions.

However, these schemes are severely constrained by the C.F.L condition, then, before to conclude on the computational efficiency we need further investigations especially for multidimensional steady-state computations. Work in progress shows that the Godunov-type schemes can be extended to two-dimensional implicit methods with efficient solution procedures.

Finally, the extension of these numerical methods to two-phase separated models (6 equations models) may be possible but it requires the preliminary study of the Riemann problem. The resolution of the Riemann problem for two-fluid models presents considerable difficulties because of mathematical complications such as the loss of hyperbolicity and the nonconservative form of the system. However, it doesn't appear unlikely to succeed; some results in this way can be found in reference 12.

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Two-phase flow shock-tube problem

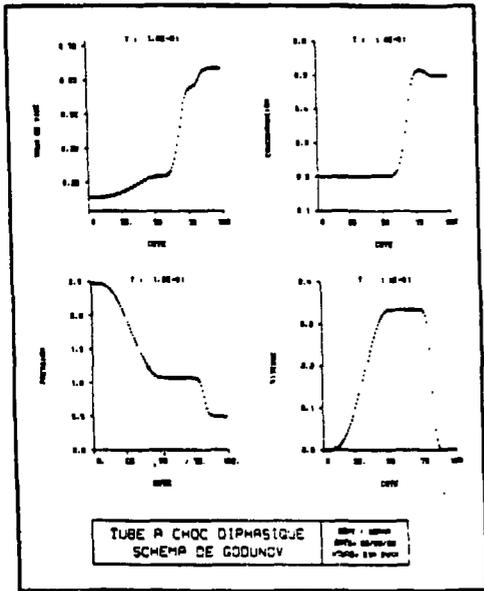


Figure 1. Godunov's scheme

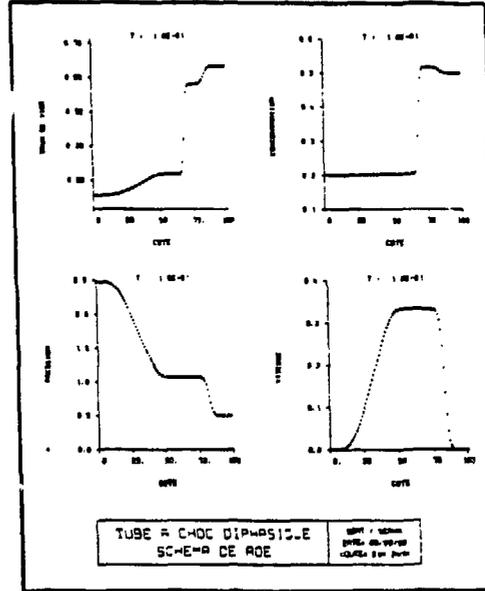


Figure 2. Roe's scheme

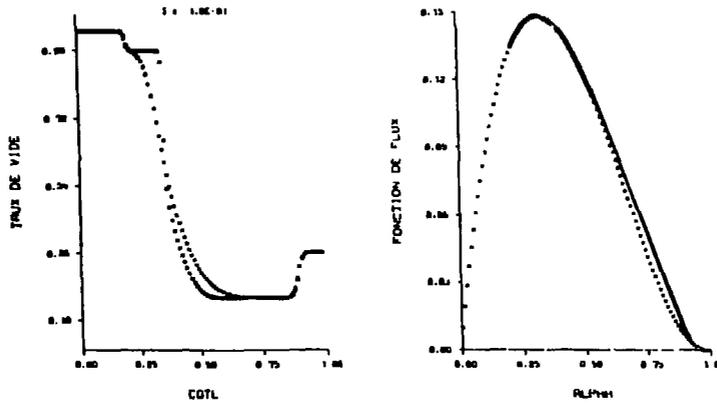


Figure 3. Comparison of Godunov and Roe's scheme on a double 2-wave.

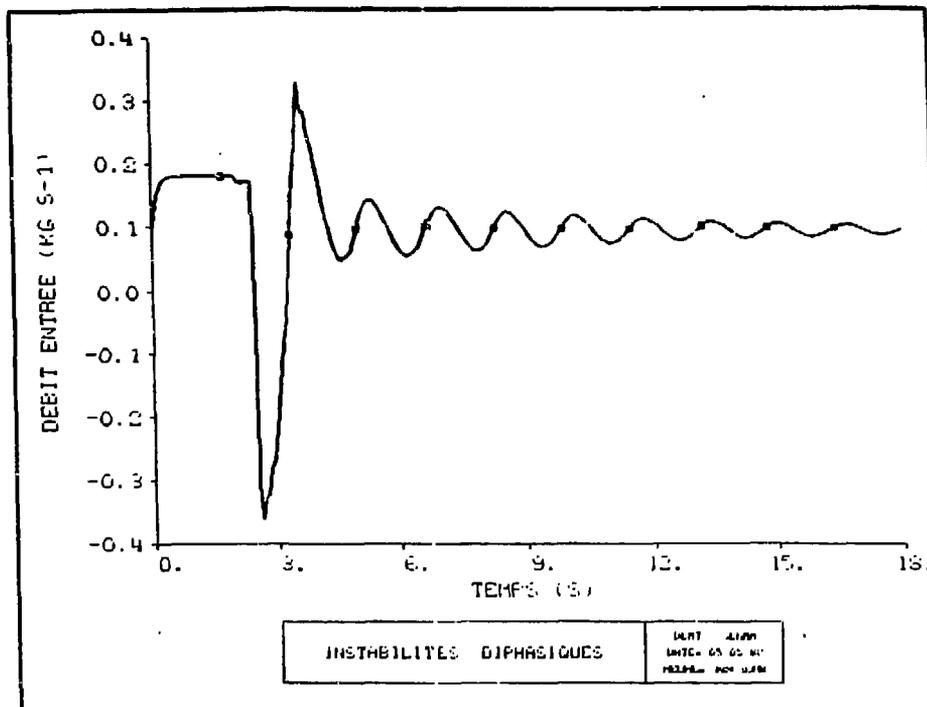


Figure 4. Two-phase flow instabilities: Inlet mass flow rate

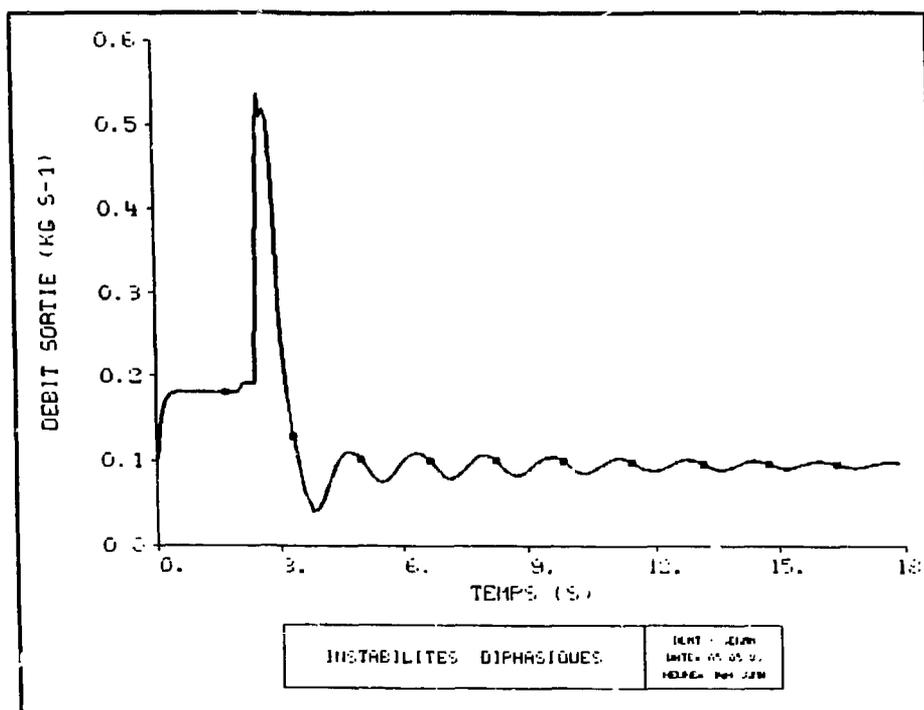


Figure 5. Two-phase flow instabilities: Outlet mass flow rate

AA