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A Mathematical and Numerical Study of Nonlinear Waves Arising in a One-Dimensional Model of a Fluidized Bed

Final Report

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1. Introduction

In sections 2-4 we present the fundamental mathematical model and the important features we have discovered during the last three years. The model presented in section 2 is typical of the set of equations studied by researchers in the past. However, a novel approach is taken here by the introduction of a stream function for the total mass flux. This is done because the differences and similarities between the one-dimensional and two-dimensional models emerge very clearly in this setting. The mathematical model is a quasilinear hyperbolic-elliptic system of partial differential equations. In one dimension the hyperbolic and elliptic parts decouple and in two dimensions they do not. As shocks and free boundaries are expected to play an important part, we also develop the jump conditions for the model in section 2.

Due to the difficulties in studying such a complicated model, it is natural to try to find simple sub-models. In our one-dimensional analysis, the kinematic model which omits particle inertia and particle phase pressure as well as fluid inertia played such a role. However, in two-dimensions it is easy to show that the kinematic model does not allow for variations in particle concentrations in the horizontal direction nor for slip between the horizontal velocity component of the gas phase and particle phase. Unlike the one-dimensional case, it appears that particle inertia plays an important role in non-trivial solutions of the two-dimensional equations. This leads to a consideration of travelling wave solutions of the full equations which we regard as the model for slugs and bubbles. Section 3 discusses the restriction of the model to travelling waves, reviews some of our past work on one-dimensional waves, and outlines our own bubble theory. This bubble theory arose from our formulation of the problem in section 2 and our experience with the one-dimensional wave.

During the 1991-92 academic year we provided salary support for a graduate student in mechanical engineering at West Virginia University. Using university equipment he is building a (one-dimensional) slugging fluidized bed. He is studying it using a high speed camera and computer analysis of the data. We intend to continue this support and ultimately compare our theory to this data.

2. The Mathematical Model

We use a continuum approach for both the particle phase and the gas phase. The derivation of these equations is found in Drew (1983).

$$\frac{\partial \alpha}{\partial t} + \nabla.(\alpha v_p) = 0 \tag{2.1}$$

$$\frac{\partial(1-\alpha)}{\partial t} + \nabla.(1-\alpha)v_g = 0 \tag{2.2}$$

$$\frac{\partial(\rho_p \alpha v_p)}{\partial t} + \nabla.(\alpha\rho_p v_p v_p) = -\alpha\nabla p_g - \nabla\alpha(p_p-p_g) - \rho_p\alpha g + B(\alpha)(v_g-v_p) \tag{2.3}$$

$$0 = -(1-\alpha)\nabla p_g - B(v_g-v_p) \tag{2.4}$$

Equations (2.1), (2.2) are the continuity equations for each phase and (2.3), (2.4) are the momentum balances. The concentration of particles by volume is denoted by α; v_p, v_g are the velocities in the particle and gas phases; ρ_p, ρ_g are the actual densities of the particles and gas; g is the acceleration due to gravity; B is the drag coefficient. Since $\rho_p >> \rho_g$, the inertia of the gas is neglected in (2.4) leaving Darcy's law.

As in Needham and Merkin (1983), Fanucci et al (1979, 1981), and Liu (1982, 1983), we are using a linear drag law, primarily because of its simplicity. The use of more realistic drag laws such as those used by Foscolo and Gibilaro (1987) is not expected to affect the qualitative behaviour of solutions. Our numerical work on a one-dimensional model supports this view. In our numerical calculations, we take (see Needham and Merkin 1983)

$$B(\alpha) = \frac{g\rho_p}{v_t}\alpha(1-\alpha)^{2-n}$$

where $n \cong 4$ and v_t is the terminal velocity of an isolated particle.

The difference between the pressures in the two phases is modelled as

$$\alpha(p_p-p_g) = \rho_p v_t^2 F(\alpha).$$

It is usually assumed that $F'(\alpha)>0$. For example, in Needham and Merkin (1983), Liu (1982, 1983), and Homsy et al (1980), F' is assumed to be a positive constant and in Fanucci et al (1979, 1981), F' exhibits rapid growth for larger particle concentrations. In this last choice for F', the physically motivated properties are that F' is small for small α and becomes infinite as α approaches a packing concentration $\alpha_p<1$. These are essentially the properties of an incompressible model.

The continuity equations are manipulated in the following manner: Adding (2.1) and (2.2) implies that the vector field $\alpha v_p+(1-\alpha)v_g$ is divergence-free. Since we will study at most problems with spatial variations in the vertical direction (z-axis) and the horizontal direction (x-axis) this constraint on $\alpha v_p+(1-\alpha)v_g$ can be satisfied by the introduction of a stream function $\psi(x,z)$ with the following properties:

$$\alpha v_{px}+(1-\alpha)v_{gx} = \frac{\partial\psi}{\partial z} \tag{2.5}$$

$$\alpha v_{pz}+(1-\alpha)v_{gz} = -\frac{\partial\psi}{\partial x}. \tag{2.6}$$

The subscripts x and z denote to the first and second components of the velocity vectors respectively. Equations (2.5) and (2.6) can then be used to eliminate v_{gx} and v_{gz} from the problem. In particular, (2.3) becomes in component form (after using (2.4) to eliminate ∇p_g)

$$\rho_p\left[\frac{\partial(\alpha v_{px})}{\partial t}+\frac{\partial(\alpha v_{px}^2)}{\partial x}+\frac{\partial(\alpha v_{px}v_{pz})}{\partial z}\right] = -\rho_p v_t^2\frac{\partial F}{\partial x}+\frac{B(\alpha)}{(1-\alpha)^2}\left[\frac{\partial\psi}{\partial z}-v_{px}\right] \tag{2.7}$$

$$\rho_p\left[\frac{\partial(\alpha v_{pz})}{\partial t}+\frac{\partial(\alpha v_{px}v_{pz})}{\partial x}+\frac{\partial(\alpha v_{pz}^2)}{\partial z}\right] = \tag{2.8}$$

$$-\rho_p v_t^2\frac{\partial F}{\partial z}+\frac{B(\alpha)}{(1-\alpha)^2}\left[-\frac{\partial\psi}{\partial x}-v_{pz}\right]-\rho_p\alpha g.$$

Assuming $\frac{\partial^2 p_g}{\partial x\partial z}=\frac{\partial^2 p_g}{\partial z\partial x}$ in (2.4) yields an equation for ψ given by

$$G(\alpha)\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial z^2}\right] = -\frac{G(\alpha)}{\alpha}\left[\frac{\partial(\alpha v_{pz})}{\partial x}-\frac{\partial(\alpha v_{px})}{\partial z}-v_{pz}\frac{\partial\alpha}{\partial x}+v_{px}\frac{\partial\alpha}{\partial z}\right] \tag{2.9}$$

$$-\left[G'(\alpha)+\frac{G(\alpha)}{(1-\alpha)}\right]\left[\frac{\partial\alpha}{\partial z}\frac{\partial\psi}{\partial z}+\frac{\partial\alpha}{\partial x}\frac{\partial\psi}{\partial x}+\frac{\partial\alpha}{\partial x}v_{pz}-\frac{\partial\alpha}{\partial z}v_{px}\right]$$

where $G(\alpha) = -\frac{B(\alpha)}{(1-\alpha)}$. It is clear that this is an elliptic equation for ψ.

Since G(0)=0, the equation is singular at $\alpha=0$. In the one-dimensional analysis ($v_{px} \equiv 0$, $\frac{\partial(\cdot)}{\partial x} \equiv 0$), ψ must satisfy Laplace's equation even where $\alpha=0$. For two space dimensions the original model only implies that $\nabla p=0$ and the behaviour of the gas is unknown (in one-dimension it must flow along the one streamline - the tube). In our present analytical and numerical work we are assuming that the flow of gas is irrotational and that ψ satisfies Laplace's equation when $\alpha=0$.

The dependent variables we study are α, v_{px}, v_{pz}, and ψ with equations (2.7), (2.8), (2.9), and (2.1). The pressure gradient and the velocity of the gas can be found from (2.4), (2.5), and (2.6).

The boundary conditions on ψ and v_p can be easily found from (2.5) and (2.6). The horizontal velocity of both phases at the vertical walls located at $x=\pm a$ is zero and, therefore, $\frac{\partial\psi}{\partial z}=0$ and $v_{px}=0$ at $x=\pm a$. Since our model contains no viscosity, we allow for slip at the walls. At the distributor plate (z=0) we assume that $v_{pz}=0$ and the volumetric flux of gas (volume per unit area per unit time) in the vertical direction equals a constant j, the flux of gas entering the distributor plate:

$$-\frac{\partial\psi}{\partial x} = j = (1-\alpha)v_{gz} \quad \text{at } z=0.$$

The same condition is imposed at the top of the bed. The boundary conditions on ψ can obviously be integrated, eliminating an arbitrary constant in the solution for ψ. This result is illustrated in Figure 1.

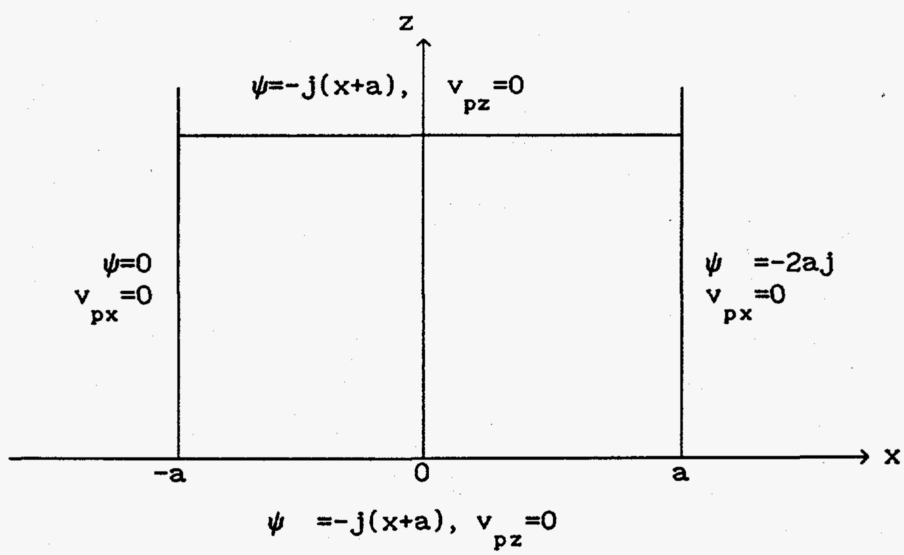

Figure 1

A reason for the introduction of the stream function is to cast the problem in such a way that our one-dimensional analysis can be easily seen as a special case and to make generalizations to two-dimensions more likely. In a one-dimensional analysis we have $\alpha=\alpha(z,t)$, $v_{pz}=v_{pz}(z,t)$, and $v_{px}\equiv 0$. Consequently, from (2.7), we must have $\frac{\partial\psi}{\partial z}\equiv 0$. This means that (2.9) reduces to Laplace's equation for ψ and, therefore, $\psi = -j(x+a)$. In one space dimension the equation for ψ does not depend on v_p or α and can be solved independently of these fields.

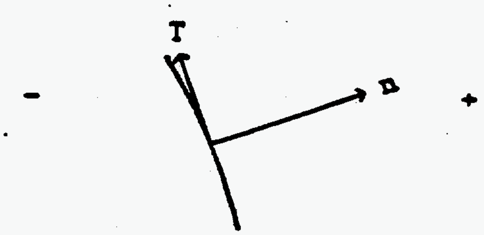

Figure 2

To complete the description of the mathematical problem we list the jump conditions. Let ± denote the two sides of the jump and n the unit vector at the jump pointing into the + region. The velocity of the jump is v_s and T is a unit tangent vector (see Figure 2). The jump conditions are calculated in the usual way from the integral form of the balance laws. Conservation of mass of particles gives

(2.10) $$\alpha^+(v_p^+ - v_s).n = \alpha^-(v_p^- - v_s).n$$

and conservation of mass of the total flux $\alpha v_p+(1-\alpha)v_g$ gives

$$(\alpha^+v_p^+ + (1-\alpha^+)v_g^+).n = (\alpha^-v_p^- + (1-\alpha^-)v_g^-).n$$

which can be expressed in terms of ψ as

(2.11) $$\nabla\psi^+.T = \nabla\psi^-.T.$$

From conservation of momentum of the particles we have

$$(2.12)\qquad [\alpha^+(v_p^+ - v_s).n]v_p^+ + v_t^2F(\alpha^+)n = [\alpha^-(v_p^- - v_s).n]v_p^- + v_t^2F(\alpha^-)n$$

and, from conservation of momentum of the gas

$$p_g^+ = p_g^-$$

or, in terms of α, v_p, and ψ,

$$(2.13)\qquad \frac{G(\alpha^+)}{(1-\alpha^+)}\left[-\frac{\partial\psi^+}{\partial n} - v_p^+.T\right] = \frac{G(\alpha^-)}{(1-\alpha^-)}\left[-\frac{\partial\psi^-}{\partial n} - v_p^-.T\right].$$

Actually, (2.13) says that the change in pressure along the discontinuity is the same on both sides; $\nabla p^+.T=\nabla p^-.T$. A special case is a bubble where $\alpha^+\equiv0$ and consequently no particles enter the bubble. Then (2.12) reduces to $F(\alpha^+)=F(\alpha^-)$. We assume $F(\alpha^+)=0$. If $F>0$ for $0<\alpha<\alpha_p$ then $\alpha^-=0$ and there is no jump in particle concentration at the bubble surface. On the other hand, if $F(\alpha)=0$ for $\alpha>0$, say, as in the incompressible case where $F(\alpha)=0$ for $0\le\alpha<\alpha_p$, then a jump in α is possible. Obviously a nonzero F provides the mechanism for a smooth transition in particle concentration at the bubble surface.

At the surface of a bubble in the case when $F(\alpha)=0$ near $\alpha=0$ (2.13) reduces to

$$(2.14)\qquad \frac{\partial\psi^-}{\partial n} = -\,v_p^-.T$$

since $G(\alpha^+=0)=0$ and $G(\alpha^-)\neq0$. An alternative form of (2.14) can be found by eliminating $\frac{\partial\psi^-}{\partial n}$ using (2.7) and (2.8) to give

$$(2.15)\qquad \frac{dv_p^-}{dt}.T = -g.T. \qquad \left[\text{Note that } \frac{d}{dt} = \frac{\partial}{\partial t} + v_{px}\frac{\partial}{\partial x} + v_{pz}\frac{\partial}{\partial z}.\right]$$

This can be found directly from (2.3) and (2.4) since $\nabla p_g=0$ inside a bubble and consequently in the incompressible case the only force acting on the particle in the tangential direction at the bubble surface is gravity. In the special case of a bubble moving with speed $s=u_B$, (2.15) can be manipulated to give the differential relationship

$$d|v_p^- - u_B|^2 = -2g\, dz' \qquad (2.16)$$

where $z'=z-u_Bt$ is the coordinate moving with the bubble (see section 3.1). Physical and mathematical arguments imply that (2.14) and (2.15) would also hold in the case $F(\alpha)>0$ if $F(\alpha)$ vanishes fast enough as α approaches zero.

The problem for α, v_{px}, v_{pz}, and ψ is a two-dimensional quasilinear hyperbolic-elliptic coupled system. At present there are no analytic results available for the study of this system. However, there has been work done on similar hyperbolic-parabolic coupled systems by Li (1987, 1988b).

3. Travelling Waves in One and Two Space Dimensions

In this section the equations describing a travelling wave moving at a constant speed in the vertical direction are developed. This is done assuming variations in two space dimensions. We continue to seek formulations that allow the results of our one-dimensional work to assist in the two-dimensional analysis. One such formulation permits us to find (or approximate) the momentum αv_p as a function of position and then to calculate α and v_p. Although not perfectly suited to this plan, the equation for evolution of momentum vorticity derived in section 3.1 allows us to make some progress. The Bernoulli equation conceived by (2.7) and (2.8) also derived in section 3.1 is the equation that then gives α as a function of position. This strategy works perfectly in one-dimension and gives us the opportunity in section 3.2 to demonstrate this approach and review our results of the last three years. Section 3.3 discusses our current and proposed research into the stability of the one-dimensional travelling wave. In section 3.4 we outline our bubble theory which is an extension to two space variables of the strategy used in section 3.2.

3.1 The equations for a travelling wave.

Let $z'=z-st$, $x'=x$, $v'_{pz}=v_{pz}-s$, and $v'_{px}=v_{px}$ denote the variables for a travelling wave moving at speed s in the vertical direction. We now look for solutions which are functions of x' and z' and independent of t directly. Equation (2.1) becomes

$$\frac{\partial(\alpha v'_{px})}{\partial x'} + \frac{\partial(\alpha v'_{pz})}{\partial z'} = 0. \tag{3.1.1}$$

As will be shown, a natural generalization of the one-dimensional analysis is to calculate the Bernoulli equation corresponding to (2.7) and (2.8). In travelling wave variables these equations can be rewritten as

$$\alpha v'_p . \nabla v'_p = -v_t^2 \nabla F - \alpha g - \frac{1}{\rho_p} \nabla p_g$$

since (3.1.1) holds. We have temporarily replaced the drag term with ∇p_g for simplicity of notation. Since

$$v'_p . \nabla v'_p = \nabla . \frac{1}{2}|v'_p|^2 - v'_p \wedge \text{curl } v'_p$$

the above equation becomes

$$\nabla . \left[\frac{1}{2}|v'_p|^2 + v_t^2 \mathcal{F}(\alpha) \right] - v'_p \wedge \text{curl } v'_p = - \frac{1}{\alpha \rho_p} \nabla p_g - g$$

where

$$\mathcal{F}(\alpha) = \int^{\alpha} \frac{F'(\alpha)}{\alpha} d\alpha.$$

To remove the quantity $v'_p \wedge \text{curl } v'_p$, the dot product of the above equation with $\frac{dr}{d\sigma}$ is calculated, where r is the position vector for a particle streamline and σ is the arclength:

$$\frac{d}{d\sigma}\left[\frac{1}{2}|v'_p|^2 + v_t^2 \mathcal{F}(\alpha) \right] = - \frac{1}{\alpha\rho_p} \nabla p_g . \frac{dr}{d\sigma} - g . \frac{dr}{d\sigma} \tag{3.1.2}$$

$(v'_p \wedge \text{curl } v'_p).\frac{dr}{d\sigma}$ vanishes since $\frac{dr}{d\sigma}$ is parallel to v'_p.

In the one-dimensional analysis $(\frac{\partial(\cdot)}{\partial x'} = 0,\ v'_{px} = 0)$ equation (3.1.1) implies that $\alpha v'_{pz} = c = $ constant. In this case there is only one streamline and it is in the vertical direction. ($\frac{dr}{d\sigma}$ = a constant unit vector in the vertical direction.) Using $v'_{pz} = c/\alpha$, (3.1.2) shows how α varies with $z'=\sigma$.

In the general two-dimensional case this simple relationship between the velocity field and particle concentration does not exist. However, a relationship does exist which can be studied by finding how the vorticity of the momentum field

$$\frac{\partial(\alpha v'_{px})}{\partial z'} - \frac{\partial(\alpha v'_{pz})}{\partial x'}$$

evolves. This equation can be found using the standard arguments applied to an inviscid fluid with variable density (see Yih 1979 page 62). The usual vorticity equation found involves the vorticity of the velocity field

$$\frac{\partial v'_{px}}{\partial z'} - \frac{\partial v'_{pz}}{\partial x'}$$

but it is easy to convert the result to momentum vorticity. This result is best stated in terms of a stream function ψ_p which automatically solves (3.1.1):

$$\frac{\partial \psi_p}{\partial z'} = \alpha v'_{px}$$

$$-\frac{\partial \psi_p}{\partial x'} = \alpha v'_{pz}.$$

The equation for momentum vorticity is

$$\text{(3.1.3)} \qquad \frac{d}{dt}\left[\frac{\partial(\alpha v'_{px})}{\partial z'} - \frac{\partial(\alpha v'_{pz})}{\partial x'}\right] = \frac{d}{dt}\left[\frac{\partial^2\psi_p}{\partial z'^2} + \frac{\partial^2\psi_p}{\partial x'^2}\right] =$$

$$2\left[\frac{\partial^2\psi_p}{\partial z'^2} + \frac{\partial^2\psi_p}{\partial x'^2}\right]\frac{d\alpha}{dt} - \frac{2}{\alpha}\frac{d\alpha}{dt}\left[\frac{\partial\psi_p}{\partial x'}\frac{\partial\alpha}{\partial x'} + \frac{\partial\psi_p}{\partial z'}\frac{\partial\alpha}{\partial z'}\right] + \frac{1}{\alpha}\frac{\partial\psi_p}{\partial z'}\frac{d}{dt}\left[\frac{\partial\alpha}{\partial z'}\right]$$

$$+ \frac{1}{\alpha}\frac{\partial\psi_p}{\partial x'}\frac{d}{dt}\left[\frac{\partial\alpha}{\partial x'}\right] + g\frac{\partial\alpha}{\partial x'}. \qquad \left[\text{Note that } \frac{d}{dt} = v'_{px}\frac{\partial}{\partial x'} + v'_{pz}\frac{\partial}{\partial z'}.\right]$$

In the calculation of the travelling wave the distributor plate is not present and the bed extends to infinity in all directions where it is uniformly fluidized with particle concentrations α_0. The boundary conditions for ψ_p come from $\alpha v'_{pz}=-\alpha_0 s$ and $\alpha v'_{px}=0$ at infinity and (2.10) at discontinuities. For example, in the case of a two-dimensional bubble $\alpha v'_p.n=0$ at the surface.

The relationship between ψ and its form in the travelling wave variables is $\psi = \psi'-sx$ which can be deduced from (2.5) and (2.6). It is easy to calculate the new problem for ψ' in terms of travelling wave variables. In (2.9), (2.11), and (2.13)-(2.15) primes are inserted and, in Figure 1, j is replaced by j-s. The dependent variables in the travelling wave problem are ψ', ψ_p, and α.

3.2 One-dimensional travelling waves.

We now review the main analytical work completed by our group on the one-dimensional waves as well as describing the direction of our current research on their stability.

In the one-dimensional analysis $v'_{px} = 0$ and $\frac{\partial(\cdot)}{\partial x'} = 0$. Equation (3.1.3) reduces to terms involving only the Laplacian of ψ_p. The obvious solution satisfying the boundary conditions is $\psi_p = \alpha_0 sx$ + arbitrary constant, giving the expected result

$$\alpha v'_{pz} = -\frac{\partial \psi_p}{\partial x'} = \alpha_0 s = c. \tag{3.2.1}$$

The solution for ψ in one space dimension has already been given and, in terms of ψ', it is

$$\psi' = -(j-s)(x'+a). \tag{3.2.2}$$

For the one-dimensional analysis it is not important whether we recognize the boundaries at $x=\pm a$ or not. This obviously becomes important in two space dimensions.

It remains to determine how α varies with $\Delta=z'$ using (3.1.2). ∇p_g can be eliminated again in favour of $v'_{gz} - v'_{pz}$ using (2.4) and these velocities can be put in terms of α using (2.5), (2.6), (3.2.1), and (3.2.2). After some manipulation, this gives

$$\frac{H(\alpha)}{\alpha^3 g}\left(c^2 - v_t^2 \alpha^2 F'(\alpha)\right)\frac{d\alpha}{dz'} = H(\alpha) + \alpha j - c - \alpha s \tag{3.2.3}$$

which is equation (6) in the paper by Ganser and Lightbourne (1991). $H(\alpha)$ is a more convenient function for analyzing the kinematics of the problem. It is defined on page 1340 with graph shown in Fig. 1 of the paper.

The analysis of (3.2.3) is presented in section 4 of that paper. We now summarize those results. Equation (3.2.3) describes a transition in α from α_1 at $z'=\infty$ to α'_2 at $z'=-\infty$. Control over α_1 and α'_2 is through the choice of s and c. The relationship between α_1 and α'_2 and the other parameters in the problem follow. The most important parameter is the concentration $\alpha=\alpha^u$ which separates (linearly) stable uniformly fluidized states with $\alpha>\alpha^u$ from unstable states with $\alpha<\alpha^u$. For $\alpha_1>\alpha^u$ there is an $\alpha_2<\alpha^u$ which depends on α_1 such that smooth transitions from α_1 to α'_2 exist as long as $\alpha'_2>\alpha_2$ and $\alpha'_2<\alpha_1$. It can be shown that as $\alpha_1 \longrightarrow \alpha^{u+}$, $\alpha_2 \longrightarrow \alpha^{u-}$. The choice of s and c which gives $\alpha'_2=\alpha_2$ is singular and instead of $\alpha(-\infty)=\alpha_2$ we have $\alpha(-\infty)=\alpha_3<\alpha_2$. Choices with $\alpha'_2<\alpha_2$ do not yield simple transitional solutions.

As discussed in section 4 of Ganser and Lightbourne (1991), the transitional solutions from α_1 to $\alpha'_2>\alpha_2$ have been known for some time. However, the solution from α_1 to α_3 is new. It also has the important property that a family of admissible shocks as shown in Fig. 2 on page 1344 of the paper exists (here $\xi=z'$). There are no admissible shocks for transitions from α_1 to $\alpha'_2>\alpha_2$. The oscillatory solutions shown in the figure clearly are conceived by the unstable nature of the solutions of the equations. In the next section we present some of our current work on stability of the travelling waves themselves.

3.3 Investigations into the stability of one-dimensional travelling waves.

Traditionally, transition solutions connect two stable equilibrium states. However, our transition solution connects the stable α_1 state to an unstable α_3 state. Fortunately, an admissible shock exists so that the α_3 state is never attained. Nevertheless, the question of stability is more interesting and delicate than in the traditional problem.

Since we are interested in stability, we must return to the one-dimensional version of the original transient equations. This can be simplified to equations (2a) and (2b) in the paper by Ganser and Lightbourne (1991). One approach taken by our group is to recast the problem in terms of α and t as the independent variables and x and αv as the dependent variables. After considerable calculation this yields an equation for αv,

$$(3.3.1) \qquad (w^2-\alpha^2 v_t^2 F')\,\frac{\partial^2(\alpha v)}{\partial t^2} + 2wz\alpha\,\frac{\partial^2(\alpha v)}{\partial\alpha\partial t} + z^2\alpha^2\,\frac{\partial^2(\alpha v)}{\partial\alpha^2}$$

$$+ \left[\frac{-g\alpha}{H(\alpha)}\,(w^2-\alpha^2 v_t^2 F') - 2wz\right]\frac{\partial(\alpha v)}{\partial t} = 0$$

where

$$w = \alpha v - \alpha \frac{\partial(\alpha v)}{\partial \alpha}$$

$$z = \frac{\partial(\alpha v)}{\partial t} - \frac{g\alpha}{H(\alpha)}(\alpha v - \alpha j - H(\alpha))$$

and two equations for x

$$\frac{\partial x}{\partial \alpha} = \frac{(w^2 - \alpha^2 v_t^2 F')}{\alpha^2 z} \tag{3.3.2}$$

$$\frac{\partial x}{\partial t} = \frac{\partial(\alpha v)}{\partial \alpha}. \tag{3.3.3}$$

The compatibility condition for (3.3.2) and (3.3.3) is (3.3.1).
The equations for the two dependent variables are now decoupled. Once $(\alpha v)(\alpha,t)$ is known then (3.3.2) and (3.3.3) can be used to find $x(\alpha,t)$. This transformation ostensibly requires that the relationships between variables is monotonic and the results based on this must be viewed in this light.

The travelling wave is now the stationary solution of (3.3.1) $(\alpha v)=\alpha s+c$. To study the linear stability of the wave connecting α_1 to α_3 we look for solutions of the form

$$(\alpha v) = \alpha s + c + u$$

where s and c have the same meaning as before. Retaining only linear terms, the equation for u is

$$0 = (c^2 - \alpha^2 v_t^2 F') \frac{\partial^2 u}{\partial t^2} + 2c\bar{z}\alpha \frac{\partial^2 u}{\partial \alpha \partial t} + \alpha^2 \bar{z}^2 \frac{\partial^2 u}{\partial \alpha^2} + \left[\frac{-g\alpha}{H(\alpha)} (c^2 - \alpha^2 v_t^2 F') - 2c\bar{z} \right] \frac{\partial u}{\partial t} \tag{3.3.4}$$

where

$$\bar{z}(\alpha) = \frac{-g\alpha}{H(\alpha)}\left[\alpha s + c - (\alpha j + H(\alpha)) \right].$$

$\bar{z}(\alpha)$ has the graph shown in Figure 3.

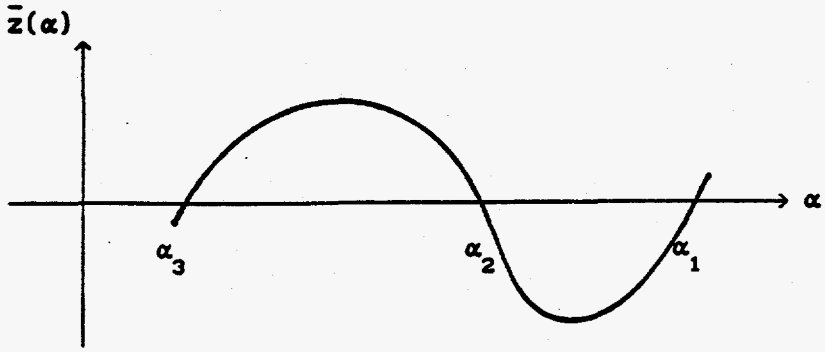

Figure 3

Equation (3.3.4) is put into canonical form by considering u as a function of α and γ where

$$\gamma = 2\left[t - c\int^{\alpha} \frac{d\alpha}{\alpha\bar{z}} \right] \tag{3.3.5}$$

yielding

$$0 = u_{\alpha\alpha} - \frac{4v_t^2F'}{\bar{z}^2}u_{\gamma\gamma} + \frac{2u_\gamma}{\alpha^2\bar{z}^2}\left[\frac{-g\alpha(c^2-\alpha^2v_t^2F')}{H(\alpha)} - c\bar{z} + c\alpha\bar{z}_\alpha \right]. \tag{3.3.6}$$

The subscripts α and γ denote partial differentiation with respect to those variables. The indefinite integral in (3.3.5) must not include α_2 as an interior point in its interval of definition since $\bar{z}(\alpha)^{-1}$ is singular at $\alpha=\alpha_2$. Thus the problem is naturally divided into the two problems $\alpha_1>\alpha>\alpha_2$ and $\alpha_3<\alpha<\alpha_2$. We shall discuss the problem with $\alpha_3<\alpha<\alpha_2$. As one might expect, this is the domain in which there is growth. Similar calculations for $\alpha_1>\alpha>\alpha_2$ suggest that perturbations decay in this domain. This forms the basis for assuming that the perturbations $u(\alpha,t)$ satisfy $u(\alpha_2,t)\equiv 0$ for $t>0$ in our analysis of $\alpha_1<\alpha<\alpha_2$.

Although we are unable to find the general solution of (3.3.6) we are able to solve a "model" equation obtained by expanding (3.3.6) for α near α_2 giving

$$(3.3.7)\qquad u_{\alpha\alpha} - \frac{4r_2^2}{(\alpha-\alpha_2)^2} u_{\gamma^*\gamma^*} + \frac{2r_2}{(\alpha-\alpha_2)^2} u_{\gamma^*} = 0$$

where

$$\gamma^* = 2t - 2r_2 \ln(\alpha_2-\alpha)$$

and

$$r_2 = \frac{v_t H(\alpha_2)\sqrt{F'(\alpha_2)}}{g\alpha_2(s-j-H'(\alpha_2))} > 0.$$

Equation (3.3.7) can be classified as a wave equation with negative damping. The general solution of (3.3.7) in terms of the original variables α and t satisfying $u(\alpha_2,t)\equiv 0$ is

$$(3.3.8)\qquad u(\alpha,t) = \exp[t/(2r_2)]\ f\left[\exp[-t/(2r_2)](\alpha_2-\alpha)\right]$$

where $f(0)=0$ and $u(\alpha,t=0)=f(\alpha_2-\alpha)$. Note that the behaviour of u as $t\rightarrow\infty$ for a fixed α depends on how fast f goes to zero as $\alpha\rightarrow\alpha_2^-$. If $u(\alpha,t=0)=o(\alpha-\alpha_2)$ then $u\rightarrow 0$ as $t\rightarrow\infty$ for fixed α. If f does not go to zero fast enough, say $f(\alpha_2-\alpha)=(\alpha_2-\alpha)^{1/2}$ then $u(\alpha,t) = \exp[t/(4r_2)](\alpha_2-\alpha)^{1/2}$ and u does not decay to zero. Note, however, that along the characteristic curve given by $\zeta=\text{constant}=t-2r_2\ln|\alpha_2-\alpha|$ any non-trivial solution of u grows.

A similar situation appears to exist for (3.3.6). A geometrical optics approximation to the behaviour of the wave front (which corresponds to the behaviour for large time) gives

$$u(\alpha,t) = G(\zeta)\ \exp\left[\int_{\alpha_3'}^{\alpha} f_8(\alpha)\ d\alpha\right],\quad \alpha_3<\alpha_3'<\alpha_2$$

where

$$\zeta = t - \int_{\alpha_3'}^{\alpha} \frac{c - v_t\alpha\sqrt{F'}}{\alpha\bar{z}}\ d\alpha$$

and $f_8(\alpha)$ depends on the coefficients in (3.3.6). Applying this technique to (3.3.7) yields (3.3.8).

The conclusions on growth are identical to those found in the model equation. For a fixed position along the travelling wave (a fixed value of α) we expect decay if f goes to zero fast enough as $\alpha \rightarrow \alpha_2^-$. Along the characteristic curve ζ=constant we expect growth. In terms of the travelling wave, ζ=constant corresponds to a position moving down the travelling wave towards the equilibrium at $\alpha=\alpha_3$. This behaviour is consistent with the fact that the equilibrium at $\alpha=\alpha_3$ is linearly unstable and yet forms a basis for considering the travelling wave with the admissible shock as a stable entity.

Another approach taken by our group, which is still in the preliminary stage, is to study the original equations directly. Both approaches support the conclusion that the travelling wave is stable in the region where $\alpha>\alpha_2$ and unstable for $\alpha<\alpha_2$. In the latter case, however, perturbations grow while moving down the travelling wave leaving behind the original wave. Numerical calculations also support this view. Figure 4 shows perturbations in two adjacent transition solutions. The perturbations can be detected beginning near α_2. Figure 5 shows a later time and how the shock absorbs the perturbations which, left on their own, grow as they approach the equilibrium $\alpha=\alpha_3$. (See section 4 for details of the numerical methods.)

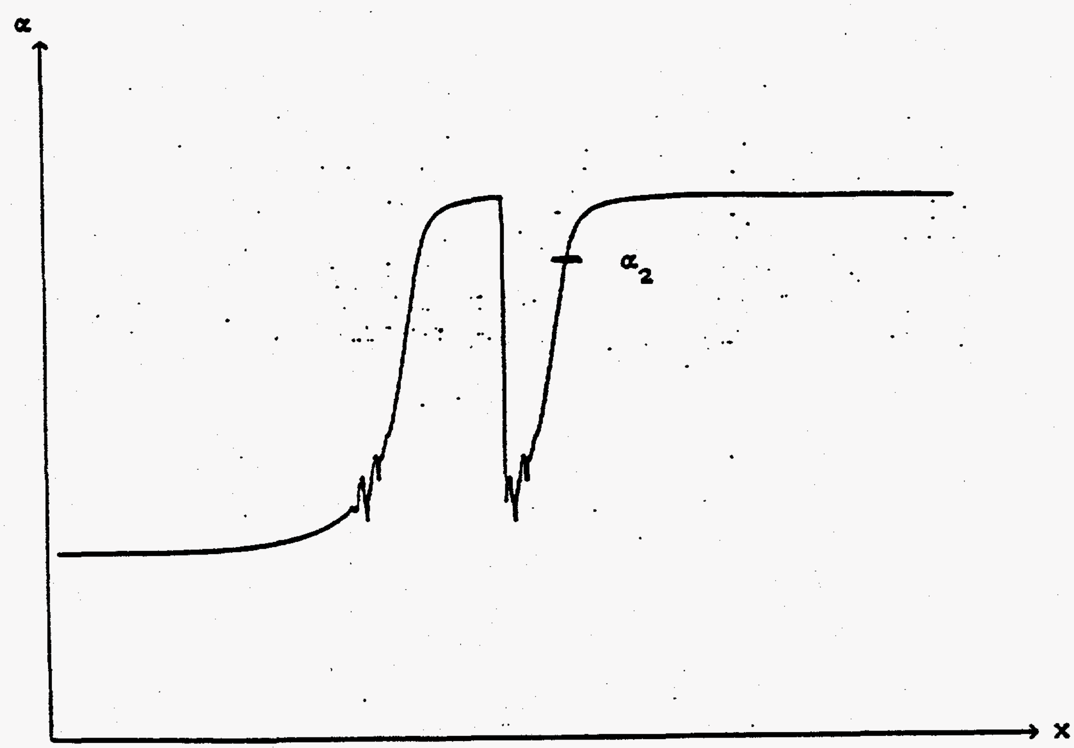

Figure 4

Further study is still necessary, in particular on the stability of the shock. The corresponding analysis for the incompressible case leads to an equation which can be classified as a backward heat equation. Remarkably we have found meaningful stable solutions due to the unusual boundaries and singularities in the coefficients of the differential equation. This will be investigated further both analytically and numerically.

We also intend to study the stability of the one-dimensional travelling wave as a solution of the two-dimensional equations. This would be an important step in the understanding of a two-dimensional bubble. A similar analysis by Clift et al (1974) was done on a motionless roof of particles over a void. Such a situation corresponds to studying the stability of one extreme member of our family of travelling waves, i.e. the case where $F\equiv0$, $\alpha_1=\alpha_p$, $\alpha_3=0$, and $s\equiv0$. Our objective is to investigate whether the stability is altered when a more realistic basic solution is used.

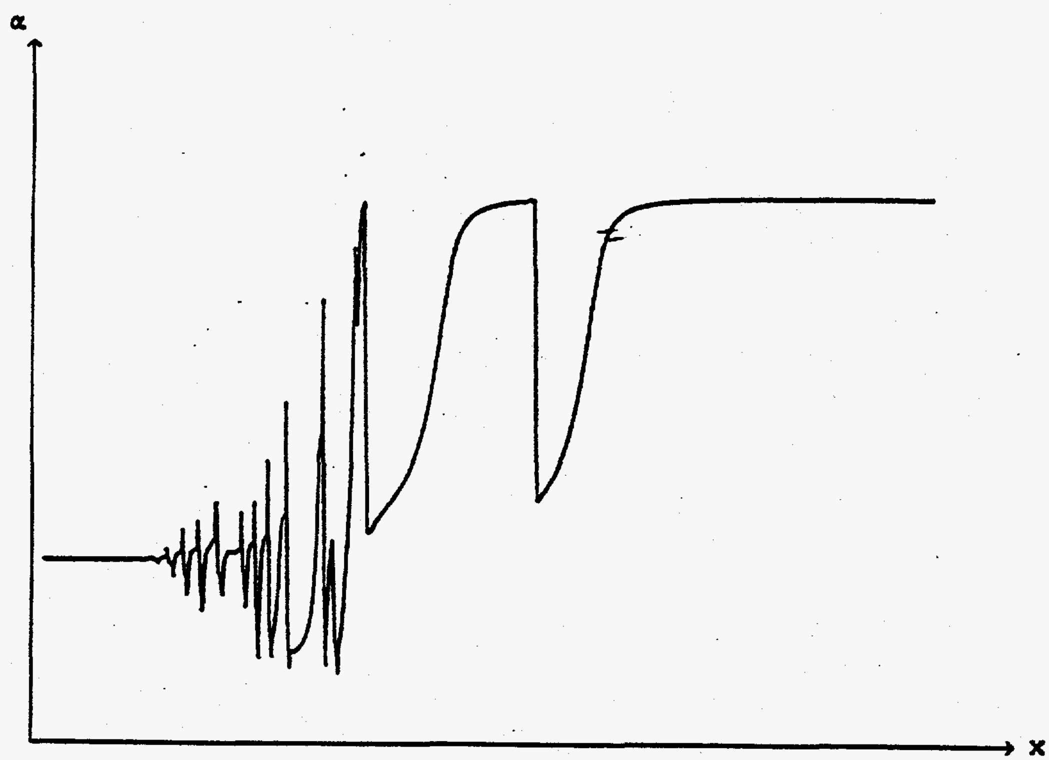

Figure 5

3.4 Travelling waves or bubbles in two dimensions.

The first theoretical work on bubbles in a fluidized bed was done by Davidson in 1961. Later work by Jackson (1963) and Murray (1965) complemented Davidson's approach. We shall first discuss Davidson's results and then introduce our work on bubbles.

Davidson's main assumption is that the particle concentration α is constant outside the bubble. Inside the bubble $\alpha=0$. As is usual in incompressible inviscid flow theory the corresponding velocity is then taken to be irrotational (see equation (3.1.3)) and hence the particle velocity field is in potential flow about the bubble. Davidson assumes the bubble is a circle of radius r_b. In terms of our stream function ψ_p with $\alpha\equiv\alpha_0$, Davidson's result is (see Figure 6)

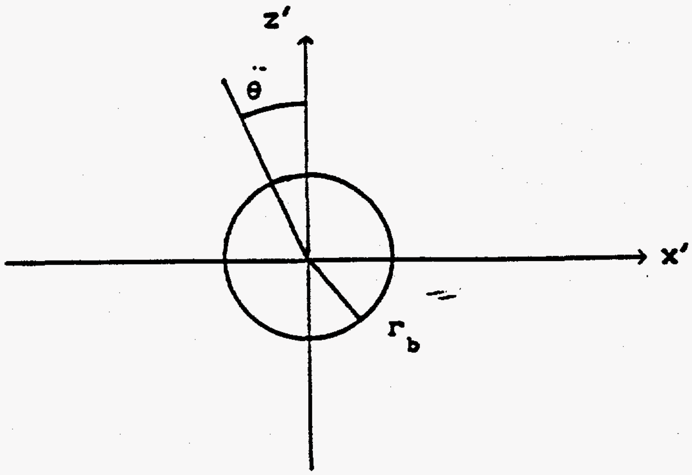

Figure 6

(3.4.1) $$\psi_p = -u_B\alpha_0\sin\theta(r-r_b^2/r)$$

(3.4.2) $$\frac{1}{r}\frac{\partial\psi_p}{\partial\theta} = \alpha_0 v'_{pr} = -u_B\alpha_0\cos\theta(1-r_b^2/r^2)$$

(3.4.3) $$-\frac{\partial\psi_p}{\partial r} = \alpha_0 v'_{p\theta} = u_B\alpha_0\sin\theta(1+r_b^2/r^2).$$

We have let $s=u_B$, the speed of the bubble.

Since $\alpha=\alpha_0$=constant also implies that the gas phase is incompressible (see equation (2.2)) a similar approach to the gas velocity is possible. However, Davidson chooses to eliminate v_p and v_g from (2.4) using (2.1) and (2.2) with $\alpha=\alpha_0$ resulting in

$$\nabla^2 p_g = 0.$$

It is easier to solve this problem than the corresponding problem for the gas potential since the pressure is known to be constant at the bubble surface and the pressure gradient far from the bubble in the uniformly fluidized bed can be found from (2.4). Knowing the pressure and the particle velocity we can then use (2.4) again to find the velocity of the gas:

(3.4.4) $$v'_{gr} = \left[\frac{j}{1-\alpha_0} - u_B \right] \cos\theta + \left[\frac{j}{1-\alpha_0} + u_B \right] \frac{r_b^2}{r^2} \cos\theta$$

(3.4.5) $$v'_{g\theta} = \left[u_B - \frac{j}{1-\alpha_0} \right] \sin\theta + \left[\frac{j}{1-\alpha_0} + u_B \right] \frac{r_b^2}{r^2} \sin\theta.$$

Using Davidson's results many general features of a bubble can be predicted, such as the existence of a "cloud" about the bubble rising in the laboratory. Collins (1965) showed that particle momentum (which Davidson ignored) can be satisfied in the tangential direction although only at the apex of the bubble, if

(3.4.6) $$u_B = \frac{1}{2} \sqrt{g r_b}.$$

Since particle momentum (3.1.2) is ignored except at the apex, discrepancies between Davidson's theory and experiment are expected especially as one moves away from the bubble apex. Consider, for example, what is the expected behaviour of the particle and gas velocities in the tangential direction at the bubble surface ($v'_{p\theta}$, $v'_{g\theta}$) and those predicted by (3.4.2) through (3.4.5). Although (3.4.2)-(3.4.5) give the same value for $v'_{p\theta}$ and $v'_{g\theta}$ ($2u_B\sin\theta$) as is necessary for the pressure to remain constant along the bubble surface, $v'_{p\theta}=v'_{g\theta}=0$ at the bottom of the bubble. However, particles at the surface are acted upon by only gravity in the tangential direction (see equation (2.1.5)) and consequently we expect $v'_{p\theta}=\sqrt{2Dg}$ at $\theta=\pi$ where $D=2r_b$ is the vertical distance the particles have fallen. Davidson and the other researchers realized this and placed no faith in the results in this region.

We now present our work on bubbles in two-dimensions which is a modified version of Davidson's theory. Briefly, we assume that the momentum αv_p instead of v_p is in potential flow. With α undetermined but αv_p known, we are now in a position to solve (3.1.2) in a manner analogous to the one-dimensional analysis. There is no a priori justification for this except that it is a natural generalization of the one-dimensional analysis.

We begin by assuming as did Davidson that α=constant in (2.9) and (3.13) and that the bubble is a circle. This implies that both ψ' and ψ_p satisfy Laplace's equation. Taking the boundary conditions into consideration gives the same problem for ψ_p as derived by Davidson. The difference is that (3.4.2) and (3.4.3) are replaced by

(3.4.7) $$\alpha v'_{pr} = -u_B \alpha_0 \cos\theta(1-r_b^2/r^2)$$

(3.4.8) $$\alpha v'_{p\theta} = u_B \alpha_0 \sin\theta(1+r_b^2/r^2).$$

The boundary conditions for ψ' are taken as (2.14) with (2.15) rewritten in current notation as (dropping minus for simplicity)

(3.4.9) $$\frac{\partial\psi'}{\partial r} = -v'_p.T.$$

Fortunately, we can calculate v'_p.T from (2.16) assuming v'_p=0 at the top of the bubble at θ=0. This gives $v'_p.T=\sqrt{2gL}$ where L is the vertical distance the particle has dropped from the bubble apex. In terms of polar coordinates, (3.4.9) becomes

(3.4.10) $$\frac{\partial\psi'}{\partial r'} = -2 \sin\frac{\theta}{2} \sqrt{gr_b} \qquad -\pi<\theta<\pi.$$

Note that the right hand side of (3.4.10) is discontinuous in physical space at the bottom of the bubble. This must be the case since particles falling from either side of the bubble along the surface meet with speed $\sqrt{4gr_b}$ at the bottom but moving in opposite directions. Since there is a flux of mass into the ray at $\theta=\pi$ on both sides this solution obviously does not satisfy conservation of mass flux, equation (2.11). However, a calculation shows that the total flux into the ray at $\theta=\pi$ ($8r_b\sqrt{gr_b}$) equals the total flux out of the bubble. Although this is not completely satisfactory it suggests a physical picture that has some merit. Applying the boundary condition

$$\frac{\partial \psi'}{\partial x'} = -(j-u_B)$$

far from the bubble (here we let $a \rightarrow \infty$) gives to within an arbitrary constant

$$\psi' = (j-u_B)\, r \sin\theta + (j-u_B)\, \frac{r_b^2}{r} \sin\theta + \frac{4\sqrt{gr_b}\, r_b^{3/2}}{r^{1/2}} \sin\frac{\theta}{2}. \tag{3.4.11}$$

With ψ' and ψ_p known, it is now possible to determine how α varies with Δ along the streamlines by using (3.1.2). This process should be considered an iterative calculation. The solution to (3.1.2) along with ψ' and ψ_p can now be substituted into (2.9) and (3.1.3) to find new approximations for ψ' and ψ_p. We shall use this iterative process to provide insight into the structure of the bubble at the bottom and its wake and to resolve the problem with ψ at $\theta=\pm\pi$.

It is possible to find exact solutions to (3.1.2) along two streamlines. We first consider the boundary of the bubble with $r=r_b$. From (3.4.7) and (3.4.8) we see $v'_{pr}=0$ and

$$v'_{p\theta} = \frac{2u_B\alpha_0}{\alpha} \sin\theta. \tag{3.4.12}$$

Substituting (3.4.12) into (3.1.2), assuming we are in the incompressible case where $\mathcal{F}(\alpha)\equiv 0$ (and thus $\alpha_0=\alpha_p$), and using $\nabla p_g \cdot \frac{dr}{d\Delta}=0$ along the boundary of the bubble yields

$$\frac{\partial}{\partial \Delta}\left[\frac{1}{2}|v'_p|^2\right] = \frac{1}{r_b}\frac{\partial}{\partial\theta}\left[\frac{2u_B^2\alpha_p^2}{\alpha^2}\sin^2\theta\right] = g\sin\theta.$$

Assuming a nonzero value for α at $\theta=0$ determines the arbitrary constant and consequently

$$\alpha = \left[\frac{2}{r_b g(1-\cos\theta)}\right]^{\frac{1}{2}} u_B \alpha_p \sin\theta \tag{3.4.13}$$

for $0<\theta<\pi$. This solution for α varies from $\alpha = 2u_B\alpha_p/\sqrt{r_b g}$ at $\theta = 0$ (using l'Hôpital's rule) to $\alpha = 0$ at $\theta = \pi$. Equation (3.4.12) now can be used to give

$$v'_{p\theta} = \sqrt{2r_b g(1-\cos\theta)}.$$

As we arranged, this gives the expected value $v'_{p\theta} = \sqrt{4r_b g}$ as $\theta \longrightarrow \pi^-$.

Since u_B is not determined at this point in our analysis neither is the value of α at the bubble apex:

$$\alpha(\theta=0) = \frac{4u_B^2\alpha_p^2}{r_b g}.$$

We note, however, that if u_B satisfies (3.4.6) then $\alpha(\theta=0)=\alpha_p$.

More insight can be found by calculating the dependence of α on arclength on the center streamline corresponding to $\theta=0$ where $s=r$. Knowing the values of v'_p and v'_g allows us to simplify (3.1.2) to

$$\text{(3.4.14)} \qquad -\frac{H(\alpha)}{g\alpha^3}\left[u_B^2\alpha_0^2(1-r_b^2/r^2)^2 - v_t^2\alpha^2F'(\alpha)\right]\frac{\partial\alpha}{\partial r} =$$

$$-\alpha j - H(\alpha) + \alpha u_B - u_B\alpha_0 - \alpha(j-u_B)\frac{r_b^2}{r^2} + u_B\alpha_0\frac{r_b^2}{r^2}$$

$$-\frac{2\alpha\sqrt{gr_b}\,r_b^{3/2}}{r^{3/2}} - \frac{2H(\alpha)u_B^2\alpha_0^2r_b^2}{g\alpha^2r^3}\left[1-\frac{r_b^2}{r^2}\right].$$

We have included the particle phase pressure $F(\alpha)$ in order to study the shock structure near the bubble. Preliminary analysis of (3.4.14) shows that there is a solution such that $\alpha(r=\infty)=\alpha_0$ and $\alpha(r=r_b)=0$. Further, as F approaches the incompressible model $\alpha(r)\longrightarrow\alpha_p$ for every $r>r_b$. This suggests that the relevant solution of (3.4.14) is $\alpha\equiv\alpha_p$ for the incompressible case. This also shows that the correct choice for the particle concentration at the top of the bubble is $\alpha=\alpha_p$ in the incompressible model and hence $u_B=\frac{1}{2}\sqrt{r_b g}$ as in the classical theory.

Assuming $F\equiv0$, Jackson (1963) constructs a theory that also introduced α as a variable. Jackson's theory allows α to vary only in the drag term in (2.3) and (2.4) ($B/(1-\alpha)$ in our model) while assuming α=constant in all the other terms. He is able to show among other things that there is a region above the bubble where α has reduced values. This is in agreement with our own bubble theory.

Murray (1965), Collins (1965), and Stewart (1968) all had their own modifications of Davidson's theory. All of these theories are different to our own bubble theory. Stewart (1968) points out that none of these classical theories individually contains the most important characteristics observed in a rising isolated bubble.

4. Numerical Methods

First we discuss some numerical techniques for solving (2.1), (2.7), (2.8), a non-homogeneous system of hyperbolic conservation laws, and (2.9), an elliptic equation for the stream function. In recent years, a large number of papers on numerical schemes for hyperbolic conservation laws has been produced by many researchers. The survey articles by Osher and Sweby (1987) and Woodward and Colella (1984) provide a comparison of some possible methods of solution. The books by LeVeque (1990) and Sod (1985) describe methods for scalar problems and systems in one and several space variables. While numerical methods for problems involving a single space variable appear to be well advanced with several techniques being capable of accurate shock resolution, the same cannot be said of methods for two-dimensional hyperbolic problems.

One of the simplest techniques for solving a problem in two space variables is dimensional splitting whereby the system is reduced to a series of one-dimensional problems. This approach conveniently enables us to make use of the Riemann solver codes which we have already developed and tested on a fluidized bed model in one space variable. There is much debate, however, about the effectiveness of dimensional splitting and its ability to deal correctly with multi-dimensional shocks which are not aligned parallel to the coordinate axes. Roe (1986, 1991) warns against its use and Shu and Osher (1989) find that it is not satisfactory for their problem. On the other hand, many authors use or suggest splitting; for example Osher and Solomon (1982), Yee (1987), and Sod (1985). Colella (1990) describes a non-split method and shows that the results compare favourably with those obtained by a split method when calculating shock reflections from an oblique surface. Yee (1987) writes "... truly two-dimensional schemes are still in the research stage. The available theory is too complicated for practical applications." Most authors solve the two-dimensional Euler equations as a test for the numerical methods. Our multi-phase flow problem presents a more severe test for the numerical methods due to the physical instabilities which are present. As a result, techniques which perform well on the Euler equations may have difficulties here.

We must also take into account a source term. We remark that, in our work in one space dimension, splitting was used without any apparent difficulties to deal with the source term (Christie, Ganser, and Sanz-Serna 1991, Christie and Palencia 1991). Other research has also concluded that splitting with respect to non-homogeneity is reasonable (LeVeque and Yee 1990, Sod 1977).

The hyperbolic system (2.1), (2.7), (2.8) can be written in the general form

$$w_t + f(w)_x + g(w)_z = b(w,\psi) \tag{4.1}$$

where $w=(\alpha,\alpha v_{px},\alpha v_{pz})^T$, and $f(w)$, $g(w)$, $b(w,\psi)$ are nonlinear functions defined by

$$f(w)=\begin{bmatrix} \alpha v_{px} \\ \alpha v_{px}^2 + v_t^2 F(\alpha) \\ \alpha v_{px} v_{pz} \end{bmatrix}, \qquad g(w)=\begin{bmatrix} \alpha v_{pz} \\ \alpha v_{px} v_{pz} \\ \alpha v_{pz}^2 + v_t^2 F(\alpha) \end{bmatrix},$$

and

$$b(w,\psi)=\begin{bmatrix} 0 \\ \dfrac{B(\alpha)}{\rho_p(1-\alpha)^2}\left(\dfrac{\partial\psi}{\partial z} - v_{px}\right) \\ \dfrac{B(\alpha)}{\rho_p(1-\alpha)^2}\left(-\dfrac{\partial\psi}{\partial x} - v_{pz}\right) - \alpha g \end{bmatrix}.$$

For the moment we assume that ψ is a known function. Later we shall discuss the numerical solution of the stream function equation (2.9).

We have two reliable and accurate computer codes for a one-dimensional fluidized bed model. One of them is based on Roe's (1981) approximate

Jacobian method and avoids non-physical shocks by means of the Harten and Hyman (1983) "entropy fix". Second order accuracy of the method is achieved by means of the flux limiting techniques described by Sweby (1984) (see the attached paper by Christie, Ganser, and Sanz-Serna 1991). The other code, derived from the exact solution of the Riemann problem, enables the method of Godunov (1959) to be used. We obtained second order accuracy in space by extending the method of Davis (1988) and applying it to the Godunov procedure (see the paper by Christie and Palencia 1991). The computer codes based on these two techniques are able to resolve shocks correctly and reproduce the slugging phenomenon. The two codes, based on different methods, give very similar solutions in numerical experiments conducted over several thousands of time steps (see Christie and Palencia 1991). This produces confidence in the results obtained.

We now describe the splitting technique. Denote the numerical solution of (4.1) at time level t_n by W^n. The Strang (1968) splitting computes the solution W^{n+1} after a time step Δt from the following algorithm:

(i) start with the known values W^n and a known stream function ψ

(ii) solve $w_t = b$ with step $\Delta t/2$

(iii) solve $w_t + f_x = 0$ with step $\Delta t/2$

(iv) solve $w_t + g_z = 0$ with step Δt

(v) repeat step (iii)

(vi) repeat step (ii) to give W^{n+1} and then compute a new ψ.

This procedure, which is formally second order accurate in time, reduces the two-dimensional system (4.1) to a series of homogeneous problems in one space variable and ordinary differential equations in time. Other types of splitting (see Mitchell and Griffiths 1980) are not expected to give substantially different results and will not be considered.

The initial value of ψ is found by solving (2.9) using the initial conditions for the concentration and velocities. The solution at each of the steps (ii)-(vi) uses the solution at the previous step as the initial value. Steps (ii) and (vi) require the solution of ODEs. If the linear drag law is used for the function $B(\alpha)$ appearing in $b(w,\psi)$ then these ODE steps can be integrated in closed form. Otherwise, a straightforward second order numerical procedure can be applied.

Steps (iii)-(v) require the solution of homogeneous systems of conservation laws in one space variable and present the most challenging aspects of the method. We propose to apply a second order Roe method to each one-dimensional system.

Differentiation of (4.1) gives

$$w_t + J(w)w_x + K(w)w_z = B \tag{4.2}$$

where J and K are the Jacobian matrices

$$J = \begin{bmatrix} 0 & 1 & 0 \\ -\lambda_+\lambda_- & \lambda_+ + \lambda_- & 0 \\ -\lambda\mu & \mu & \lambda \end{bmatrix} \quad \text{and} \quad K = \begin{bmatrix} 0 & 0 & 1 \\ -\lambda\mu & \mu & \lambda \\ -\mu_+\mu_- & 0 & \mu_+ + \mu_- \end{bmatrix}$$

whose eigenvalues are $\lambda = v_{px}$, $\lambda_\pm = v_{px} \pm \sqrt{F'}$ and $\mu = v_{pz}$, $\mu_\pm = v_{pz} \pm \sqrt{F'}$ respectively. The Roe approximate Jacobians are expressed in a similar manner in terms of their averaged eigenvalues $\bar{\lambda} = \bar{v}_{px}$, $\bar{\lambda}_\pm = \bar{v}_{px} \pm \bar{c}$, $\bar{\mu} = \bar{v}_{pz}$, and $\bar{\mu}_\pm = \bar{v}_{pz} \pm \bar{c}$ where the Roe averaged velocities are given by

$$\bar{v}_{px} = \frac{\sqrt{\alpha_R}\, v_{pxR} + \sqrt{\alpha_L}\, v_{pxL}}{\sqrt{\alpha_R} + \sqrt{\alpha_L}} \quad \text{and} \quad \bar{v}_{pz} = \frac{\sqrt{\alpha_R}\, v_{pzR} + \sqrt{\alpha_L}\, v_{pzL}}{\sqrt{\alpha_R} + \sqrt{\alpha_L}}.$$

The subscripts L and R respectively denote the left and right constant states in adjacent computational cells which are assumed by the method. The averaged speed of sound is given by

$$\bar{c}^2 = (F_R - F_L)/(\alpha_R - \alpha_L)$$

with a suitable modification to account for near equal concentrations over two adjacent cells. The construction of the matrices

$$P = \begin{bmatrix} 0 & 1 & 1 \\ 0 & \bar{\lambda}_- & \bar{\lambda}_+ \\ 1 & \bar{\mu} & \bar{\mu} \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} 0 & 1 & 1 \\ 1 & \bar{\lambda} & \bar{\lambda} \\ 0 & \bar{\mu}_- & \bar{\mu}_+ \end{bmatrix}$$

whose columns are the eigenvectors of $\bar{J}$ and $\bar{K}$ respectively then easily allows the systems appearing in steps (iii)-(v) of the algorithm to be uncoupled. This is seen by premultiplying the equation in steps (iii) and (v) by P^{-1} and in step (iv) by Q^{-1} and using $P^{-1}\bar{J}P = \mathrm{diag}(\lambda, \lambda_-, \lambda_+)$ and $Q^{-1}\bar{K}Q = \mathrm{diag}(\mu, \mu_-, \mu_+)$. The uncoupled equations are then discretized by the second order procedure described in Christie, Ganser, and Sanz-Serna (1991).

To complete the algorithm, ψ must also be calculated. The stream function equation (2.9) can be written in the form

$$c_1 \frac{\partial^2\psi}{\partial x^2} + c_2 \frac{\partial\psi}{\partial x} + c_3 \frac{\partial^2\psi}{\partial z^2} + c_4 \frac{\partial\psi}{\partial z} + c_5 = 0 \tag{4.3}$$

where the c_i terms (i=1 to 5) are defined in an obvious manner from (2.9). Due to the coupling of ψ in the system (4.1), (4.3), either an iterative procedure must be used to determine ψ or else ψ must be assigned the known values found in each cell from the previous time step to allow $b(w,\psi)$ to be constructed. In the splitting algorithm described earlier, the latter technique will be adopted.

To compute new values of ψ a splitting procedure is also possible via the inclusion of an artificial time derivative. Therefore, we can seek steady state solutions of

$$c_1 \frac{\partial^2\psi}{\partial x^2} + c_2 \frac{\partial\psi}{\partial x} + c_3 \frac{\partial^2\psi}{\partial z^2} + c_4 \frac{\partial\psi}{\partial z} + c_5 = -\psi_\tau. \tag{4.4}$$

Note that c_1 and c_3 are always negative so that the minus sign must appear on the right hand side of (4.4). Equation (4.4) can be solved as the split scheme

$$c_1 \frac{\partial^2\psi}{\partial x^2} + c_2 \frac{\partial\psi}{\partial x} + \frac{1}{2} c_5 = -\frac{1}{2} \psi_\tau$$

$$c_3 \frac{\partial^2\psi}{\partial z^2} + c_4 \frac{\partial\psi}{\partial z} + \frac{1}{2} c_5 = -\frac{1}{2} \psi_\tau$$

where each equation is solved in turn over a $\Delta\tau/2$ step by fully implicit finite differences. Several discretization methods will be considered for both the ψ derivatives and the derivatives contained in the coefficients. The need for upwind finite differencing or upwind finite elements will depend on the relative sizes of the coefficients of the first and second derivatives of ψ (see Christie, Griffiths, Mitchell, and Zienkiewicz 1976). Convergence to the steady state solution is assumed when the maximum norm of the difference between solutions at successive time levels is less than a prescribed tolerance. Preliminary indications are that this technique gives rapid convergence with the steady-state being achieved in one or two steps.

It is also possible to extend to two space dimensions the modification of the Davis (1988) method described by Christie and Palencia (1991). The method is centered in space and possesses second order accuracy in space and in time. For the homogeneous version of equation (4.1) the method has the form

$$(4.5) \qquad W_{ij}^{n+1/2} = W_{ij}^{n} - \frac{\lambda}{2}\left[f(W_{ij}^{n}+S_{ij}) - f(W_{ij}^{n}-S_{ij})\right] - \frac{\mu}{2}\left[g(W_{ij}^{n}+T_{ij}) - g(W_{ij}^{n}-T_{ij})\right]$$

$$W_{ij}^{n+1} = W_{ij}^{n} - \lambda\left[\tilde{f}(W_{ij}^{n+1/2}+S_{ij},\ W_{i+1j}^{n+1/2}-S_{i+1j}) - \tilde{f}(W_{i-1j}^{n+1/2}+S_{i-1j},\ W_{ij}^{n+1/2}-S_{ij})\right] - \mu\left[\tilde{g}(W_{ij}^{n+1/2}+T_{ij},\ W_{i+1j}^{n+1/2}-T_{i+1j}) - \tilde{g}(W_{i-1j}^{n+1/2}+T_{i-1j},\ W_{ij}^{n+1/2}-T_{ij})\right]$$

where S_{ij}, T_{ij} are flux limiters, $\tilde{f}$, $\tilde{g}$ are numerical fluxes, and $\lambda=\Delta x/\Delta t$, $\mu=\Delta z/\Delta t$ are the mesh ratios. Davis (1988) suggests a form for S_{ij} and, in the one-dimensional case, this choice led to small oscillations around shocks. In Christie and Palencia (1991) this problem was resolved by replacing the Davis flux limiter by the minmod limiter. The numerical fluxes can be substituted by the true flux when the exact solution of the Riemann problem is used.

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