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ON THE "EARLY-TIME" EVOLUTION OF VARIABLES RELEVANT TO TURBULENCE MODELS FOR THE RAYLEIGH-TAYLOR INSTABILITY

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ABSTRACT

We present our progress toward setting initial conditions in variable density turbulence models. In particular, we concentrate our efforts on the BHR turbulence model [1] for turbulent Rayleigh-Taylor instability. Our approach is to predict profiles of relevant variables before fully turbulent regime and use them as initial conditions for the turbulence model. We use an idealized model of mixing between two interpenetrating fluids to define the initial profiles for the turbulence model variables. Velocities and volume fractions used in the idealized mixing model are obtained respectively from a set of ordinary differential equations modeling the growth of the Rayleigh-Taylor instability and from an idealization of the density profile in the mixing layer. A comparison between predicted profiles for the turbulence model variables and profiles of the variables obtained from low Atwood number three dimensional simulations show reasonable agreement.

INTRODUCTION

The Rayleigh-Taylor (RT) instability is an interfacial fluid instability that leads to turbulence and turbulent mixing. It occurs when a light fluid is accelerated into a heavy fluid [2, 3] because of misalignment between density and pressure gradients. It is characterized by the Atwood number, $A=\left(\rho_h-\rho_l\right)/\left(\rho_h+\rho_l\right)$, that describes the density contrast between the heavy (h) and light (l) fluid. The Rayleigh-Taylor instability plays a key role in a wide variety of naturally occurring events such as supernovae explosions [4], salt dome formation [5], atmospheric inversions, as well as in technological applications such as heat exchangers and sprays in internal combustor [6] or in the implosion phase of Inertial Confinement Fusion (ICF) [7]. Traditional research in turbulence assumes that turbulent flows have no memory of the initial conditions, and turbulence quickly develops to a universal self-similar state. However, recent research has established that the growth of the turbulent Rayleigh-Taylor instability depends on initial conditions [8, 9]. This important finding offers an opportunity for turbulence control, which could be profitable on the condition that turbulence models can be started with the proper initial conditions.

The overall objective of this research is to provide a rational basis for initial conditions in turbulence models. We seek to predict profiles of relevant variables before the fully turbulent regime and use them as initial conditions for the turbulence model. In this paper, we expose our approach and illustrate the performance of our model in the case of a low Atwood number Rayleigh-Taylor instability. In the next section, we present the variables we want to model and our strategy to model them. The three following sections present the details of the procedure to determine the turbulence model variables' profiles and comparisons with numerical simulations. Finally, the concluding section provides a brief summary of the results and a discussion.

TURBULENCE MODEL VARIABLES

We consider the Besnard, Harlow and Rauenzhan (BHR) turbulence model [1]. Designed for variable density turbulence, the BHR turbulence model is a well-suited model for studies of turbulent Rayleigh-Taylor instability. In this single-point turbulence transport model, kinetic energy, k, normalized mass flux, $\vec{a}$, density-specific volume correlation, b, turbulence length scale, S, and turbulent viscosity, ν_t, are the key variables that need to be initiated for each simulation. These variables are defined by:

$$k = \frac{1}{2}\overline{u_i' u_i'} \tag{1}$$

$$a_i = \frac{\overline{\rho' u_i'}}{\overline{\rho}} \tag{2}$$

$$b = -\overline{\rho' v'} \tag{3}$$

$$S = \frac{k^{3/2}}{\varepsilon} \tag{4}$$

$$\nu_t = C_\mu k^{1/2} S \tag{5}$$

where, u_i' is the fluctuation of velocity component i, ρ' is the density fluctuation, $\overline{\rho}$ is the average density, v' is the specific volume fluctuation, ε is the turbulent kinetic energy dissipation and C_μ a constant coefficient. Turbulence model variables are typically set up across the computing domain as a single value representative of the problem of interest. These values are usually determined by calibration runs, results from experiments or scaling arguments. Instead, we propose to provide the turbulence model with a profile for each of these variables. The advantages of having an initial profile are two-fold: first, the profiles depend on the initial conditions that drive the flow to turbulence and second, the turbulence model benefits from a local characterization of the flow. In the context of turbulent Rayleigh-Taylor mixing, we obtain the initial profiles for the turbulence model variables following this simple procedure:

1. Predict heights and velocities of the bubbles and spikes.
2. Predict the fluids volume fraction profiles as functions of the bubble and spike heights.
3. Predict the initial profiles of the turbulence model variables as functions of the bubbles and spikes velocities and the fluids volume fraction profiles.

BUBBLE AND SPIKE PREDICTION

A reasonably successful model that describes the growth of single mode RT instability from the exponential growth rate given by linear stability analysis until the nonlinear terminal bubble (blob of light fluid penetrating into the heavy fluid) velocity is that of Goncharov [10]. The Goncharov model is a potential flow model, based on an extension of Layzer's theory for $A=1$ [11]. Consider two incompressible fluids, the heavy fluid sitting on top of the light one. In a three-dimensional axisymmetric geometry, the interface between the two fluids is approximated near the tip of the bubble by:

$$\eta(x,t) = \eta_0(t) + \eta_2(t) r^2 \tag{6}$$

where η_0 is the bubble's amplitude. The assumption is made that the fluids are irrotational in the vicinity of the bubble tip. As a consequence, Goncharov [10] defined velocity potentials as:

$$\phi^h = a_1(t) J_0(\widetilde{k} r) e^{-\widetilde{k} z} \tag{7}$$

$$\phi^l = b_1(t) J_0(\widetilde{k} r) e^{\widetilde{k} z} + b_2(t) z \tag{8}$$

where $\phi^{h/l}$ is the potential of the heavy/light fluid, J_0 is the Bessel function of order 0, $\widetilde{k}$ is the wave number of the single mode initial perturbation, $a_1 = -\frac{\dot{\eta}_0}{\widetilde{k}}$, $b_1 = \frac{\dot{\eta}_0}{\widetilde{k}} \frac{\widetilde{k} + 8\eta_2}{\widetilde{k} - 8\eta_2}$ and $b_2 = \frac{16\dot{\eta}_0 \eta_2}{8\eta_2 - \widetilde{k}}$. Upon substitution of the velocity potentials in the equations describing the conditions at the fluids interface and expanding them to the second order in r, one obtains a set of ordinary differential equations governing the dynamics of the tip of the RT bubbles until late in the nonlinear regime ($\eta_0(t) < \lambda$, where λ is the wavelength of the perturbation):

$$\eta_2 = -\frac{\widetilde{k}}{8} + \left[\frac{\widetilde{k}}{8} + \eta_2(0)\right] e^{-2\widetilde{k}[\eta_0 - \eta_0(0)]} \tag{9}$$

$$\alpha_1 \ddot{\eta}_0 + \alpha_2 \dot{\eta}_0^2 + A g \eta_2 = 0 \tag{10}$$

where

$$\alpha_1 = \frac{\widetilde{k}^2 - 4A\widetilde{k}\eta_2 - 32A\eta_2^2}{4(\widetilde{k} - 8\eta_2)} \tag{11}$$

$$\alpha_2 = \widetilde{k}^2 \frac{(5A-4)\widetilde{k}^2 + 16(2A-3)\widetilde{k}\eta_2 + 64A\eta_2^2}{8(\widetilde{k} - 8\eta_2)^2} \tag{12}$$

The set of equations governing the dynamics of the tip of the RT spike (blob of heavy fluid penetrating into the light fluid) is obtained from equations $(9)-(12)$ by substituting $\eta \to -\eta$, $A \to -A$, and $g \to -g$. According to figure 3 in Goncharov's publication [10], this nonlinear model captures with some success the penetration of the bubble for $0 \le A \le 1$, but fails to predict accurately the penetration of the spike for $A \ge 0.4$ [10, 12].

Based on the Goncharov model for single mode RT problems, we build a multimode model defined by:

$$h_{b/s}(t) = \max_{\tilde{k}}\left(h_{b/s,\tilde{k}}(t)\right) \qquad (13)$$

where $h_{b/s}(t)$ is the height of the bubbles/spikes front at time t and $h_{b/s,\tilde{k}}(t) = \left|\eta_{0,\tilde{k}}^{b/s}(t) - \eta_{0,\tilde{k}}^{b/s}(0)\right|$ is the height of the bubble/spike generated by a single mode initial perturbation of wave number k at time t. Equation (13) simply models the height of the bubbles/spikes front of a multimode RT growth as the height of the highest bubble/spike at a given time if each mode in the initial spectrum were to grow isolated from one another. Therefore, this model does not take into account the mode coupling phenomenon. This is a point of current investigation. Velocities of spikes and bubbles fronts, $v_{b/s}$, are obtained by taking a time derivative of their respective heights ($v_{b/s} = dh_{b/s}/dt$) given by the multimode model.

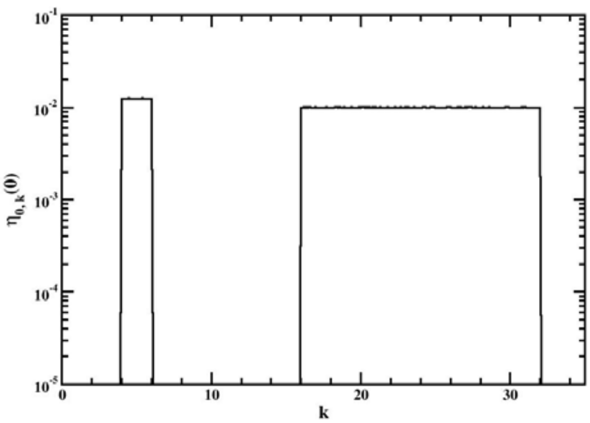

Figure 1. Initial amplitude spectrum.

Figure 1 shows the initial perturbation spectrum we choose to evaluate the overall performance of our method for predicting initial profiles of the turbulence model variables. This type of banded initial perturbation spectrum is of interest because the growth rate of the instability is modified at "late-time" under the influence of the low wave number band [9] that has slower initial growth rate. It is a valuable and challenging study case for the influence of initial conditions. We compare profiles obtained by our ODE-based method with "exact" profiles generated by a three-dimensional finite volume solver, RTI3D [13, 14]. RTI3D is an incompressible three-dimensional code that solves Euler equations and uses numerical dissipation as an artificial viscosity that smoothes out sharp gradients characteristic of Euler equations solutions. Codes that use this type of numerical techniques are referred to as MILES (Monotone Integrated Large Eddy Simulation) codes, and have proven to be particularly effective in simulation of flows with

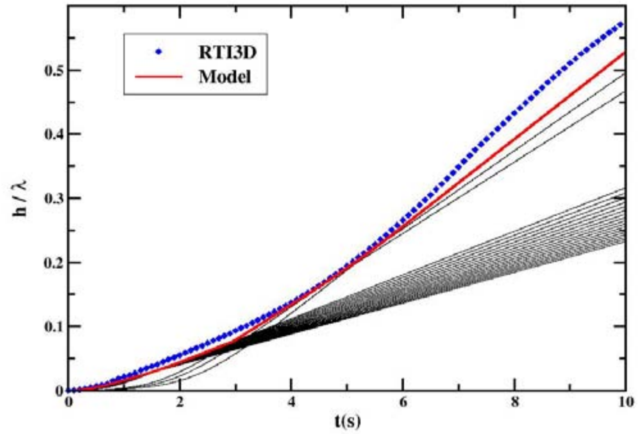

Figure 2. Height of the bubbles front as a function of time predicted by the multimode model and RTI3D simulation. Black solid lines are heights of single mode bubbles as predicted by Goncharov's model [10] for the modes composing the initial perturbation spectrum. $A = 0.01$, $g = 40$, and $\lambda = 2\pi$ is the width of the computational domain.

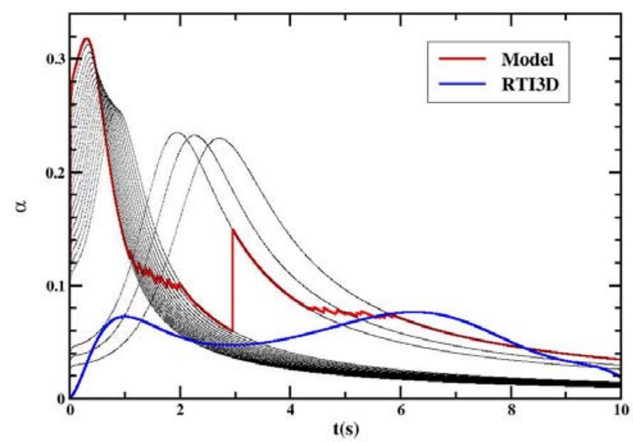

Figure 3. Growth rate, α, as defined by Ristorcelli and Clark [18] as a function of time. Black solid lines are growth rate of single mode bubbles for modes composing the initial perturbation spectrum.

discontinuities such as Rayleigh-Taylor instabilities [8, 9, 12, 15-17]. Simulations are performed at low Atwood number, $A = 0.01$, so that our method remains in its domain of validity, and with a constant acceleration of $g = 40 m/s^2$ to reach an advanced state of transition to turbulence in a relatively short physical time.

Figure 2 illustrates the performance of our multimode model for bubbles front prediction at low Atwood number. For clarity, we do not show the evolution of the spikes front as it is almost perfectly symmetric to the bubbles front evolution because of a low Atwood number. We can see in figure 2 that at all time the bubbles front in the RTI3D simulation is higher than the one from our multimode model. This discrepancy in height is due to the lack of a model for mode coupling in our current multimode model. Interactions between nearby modes, in particular superposition of modes, increase the overall height of the bubbles front. At about $t = 3s$, our multimode model predicts that bubbles associated with the low wave number band takes the lead of the bubbles front. This event is characterized by a change of slope in the curve given by our model. This significant change in dynamics is seen more clearly in figure 3 that shows a jump in the bubbles front growth rate at about $t = 3s$. The corresponding change in growth rate in the RTI3D simulation occurs more smoothly and peaks later, at about $t = 6s$,. The smooth evolution is due to mode interactions that progressively fill the entire spectrum (not taken into account in our model), such that modes that lead the bubbles front are consecutive modes. Addition of the generated low wave numbers to those existing in the initial perturbation spectrum produces this "extra kick" in the growth rate of the bubbles front observed around $t = 6s$ in the RTI3D simulation. To summarize, figure 2 and 3 show that although incomplete our multimode model captures in a reasonable fashion the evolution of the height of bubbles and spikes fronts at low Atwood number. Discrepancy at very early time between the growth rates predicted by the model and RTI3D simulation is grossly amplified because of the relatively coarse grid (64x64x128 grid cells for a domain of size 2π x 2π x 4π) used for this study.

VOLUME FRACTION PROFILE

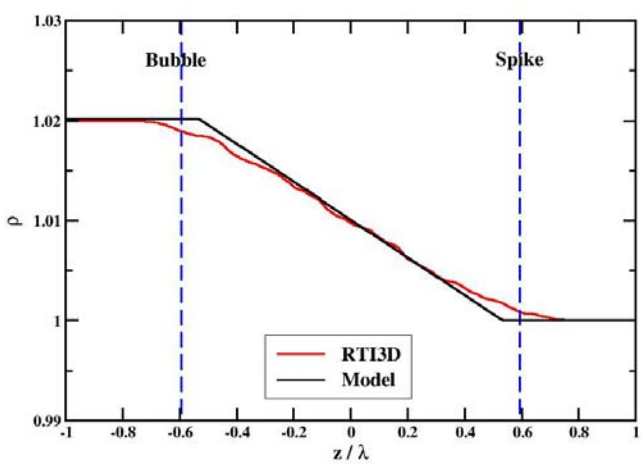

Figure 4. Density profiles in the vertical direction predicted by the model and RTI3D simulation. Vertical dashed lines indicate bubbles and spikes fronts as predicted by RTI3D, and $\lambda = 2\pi$ is the width of the computational domain.

We consider volume fraction, $f_{h/l}$, i.e. non-dimensional density, defined by:

$$\begin{cases} f_l = \dfrac{\rho - \rho_h}{\rho_l - \rho_h} \\ f_h = \dfrac{\rho - \rho_l}{\rho_h - \rho_l} \end{cases} \tag{14}$$

We assume the volume fraction is distributed in a linear fashion inside the mixing layer. To hold into account the asymmetry between the bubbles and spikes penetrations that appears with increasing Atwood number, we take the volume fraction as piecewise linear between the bubbles or spikes front and the position of the initial perturbation. Placing the initial perturbation at $z = 0$, the volume fraction profile for the heavy fluid is defined by:

$$\begin{cases} f_h = 0 & if \quad z < -h_s \\ f_h = 0.5\dfrac{z + h_s}{h_s} & if \quad -h_s \le z < 0 \\ f_h = 0.5\dfrac{z}{h_b} + 0.5 & if \quad 0 \le z \le h_b \\ f_h = 1 & if \quad z > h_b \end{cases} \tag{15}$$

The light fluid volume fraction profile is:

$$f_l = 1 - f_h \tag{16}$$

Figure 4 shows a comparison between the density profiles obtained with use of the idealized volume fraction profiles and RTI3D simulations. The density is computed from the volumes fraction profiles using the relation:

$$\rho = f_l \rho_l + f_h \rho_h \tag{17}$$

The modeled density profile matches well the density profile given by the RTI3D simulation. This simple description of the volume fraction profile as a piecewise linear function of the position in the RT mixing layer seems to hold on a large range of Atwood numbers. Indeed, at $A = 0.5$, the density profile at different stage of the evolution of the multimode RT instability always display the nearly piecewise linear shape between the density of the heavy and light fluid [19].

TWO-FLUID MODEL

We choose to use a two-fluid model [20] to predict the profiles of the turbulence model variables as functions of the mixing layer width, the velocities of the bubbles and spikes fronts and the volume fraction distribution. This model is based on an idealization of the mixing interface between two interpenetrating fluids. Following the two-fluid model, fluctuating quantities at a given altitude can be expressed as deviations from the corresponding average quantities at that same altitude, when moving horizontally within the mixing layer. For example, one can express the density fluctuation, ρ', as $\rho_h - \overline{\rho}$ or $\rho_l - \overline{\rho}$ depending on whether we are in the heavy or the light fluid, where $\overline{\rho} = f_h\rho_h + f_l\rho_l$. Similarly, the velocity fluctuation u_i' can be expressed by either $(u_h - \overline{u})_i$ or $(u_l - \overline{u})_i$ depending on whether we are in the heavy or the light fluid, where $\overline{u}_i = (f_h u_h + f_l u_l)_i$, and u_h and u_l are averaged velocities of respectively the heavy fluid and the light fluid at a given altitude in the mixing layer. Upon substitution of these expressions in equations $(1)-(3)$ and some algebra, it is found [20]:

$$k = C_k \frac{3}{2}\left(\vec{v}_b - \vec{v}_s\right)^2 \frac{f_h f_l \rho_h \rho_l}{\left(f_h\rho_h + f_l\rho_l\right)^2} \qquad (18)$$

$$a_z = C_{a_z} \frac{f_h f_l}{f_h\rho_h + f_l\rho_l}\left(\rho_h - \rho_l\right)\left(\vec{v}_s - \vec{v}_b\right) \qquad (19)$$

$$b = C_b \frac{f_h f_l \left(\rho_h - \rho_l\right)^2}{\rho_h\rho_l} \qquad (20)$$

where C_k , C_{a_z}, and C_b are coefficients equal to 1 at this stage of our research. Equation (18) assumes isotropy, which is not valid for Rayleigh-Taylor instabilities but is necessary at this point in our approach since we only know of vertical velocities of the bubbles and spikes fronts. The formulation for S is motivated by the relation $k^2/\varepsilon = k^{1/2}S = D_T$, where D_T is the turbulent diffusivity. In a self-similar state and at low Atwood number, the bubbles/spikes front evolves as $h_{b/s} = \alpha A g t^2$, hence the relation $v_b = v_s = 2\alpha A g t$ for velocities. We then substitute fronts velocities in equation (18), and, using D_T, we can write a self-similar equation for ε, $\varepsilon = C_\varepsilon A^2 g^2 t$ where $C_\varepsilon = f(f_h, f_l, \rho_h, \ldots)$. Finally, using equation (4) and $h_b + h_s = 2\alpha A g t^2$, we obtain:

$$S = C_S\left(h_b + h_s\right)\left(4 f_h f_l\right)^{1/2} \qquad (21)$$

where C_s is a coefficient equal to 1 at this point.

Figures 5 - 7 show profiles for the turbulence model variables predicted by the two-fluid model and by RTI3D simulations at a late time in transition toward fully developed turbulence. Overall, the two-fluid model offers reasonable

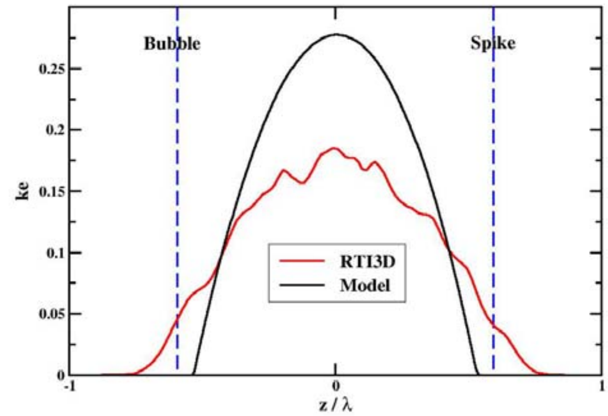

Figure 5. Kinetic energy profiles in the vertical direction as predicted by the model and RTI3D simulation. Vertical dashed lines indicate bubbles and spikes fronts as predicted by RTI3D, and $\lambda = 2\pi$ is the width of the computational domain

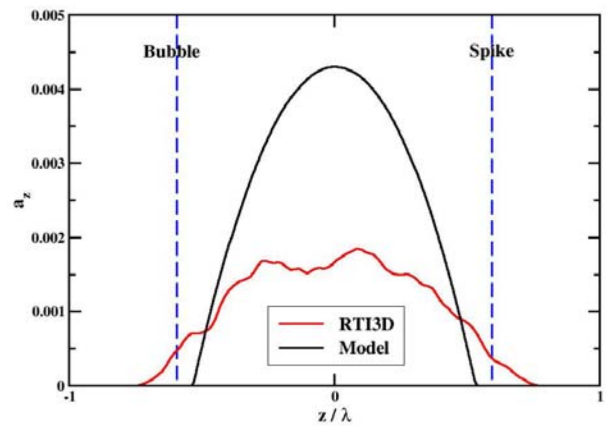

Figure 6. Normalized mass flux profiles in the vertical direction as predicted by the model and RTI3D simulation. Vertical dashed lines indicate bubbles and spikes fronts as predicted by RTI3D, and $\lambda = 2\pi$ is the width of the computational domain.

predictions of the turbulence variables profiles at the time of interest within the mixing layer at a low Atwood number. All predicted initial profiles display greater maximum values than the initial profiles obtained by numerical simulation, but they remain roughly of the same order of magnitude. Variables k and a_z are predicted with good accuracy. In the mixing layer, the assumption that the average velocity of the light/heavy fluid is about that of the bubbles/spikes front seems to be a valuable hypothesis. This hypothesis has been verified for the light fluid in the case of single mode RT instability [12]. Improvement on k and a_z could be done if one could model the average velocity profiles for the heavy and light fluid in the mixing layer. Variable b is the one that display the largest discrepancy with the numerical simulation results, figure 7. For this variable, the idealized piecewise linear volume fractions might be too simplistic to give an accurate quantitative description in this model, although it allows for a precise description of the average density profile. Also, the two-fluid model is a highly idealized description of the mixing process between two fluids. Our model does not take into account viscosity and important mechanisms such as diffusion and mode coupling are still lacking. Addition of more physics in the model as we move forward in our research for should improve prediction of the profile of variable b quantitatively and qualitatively. We cannot compare the profile of variable S predicted by our model with a profile from RTI3D. Indeed, one cannot have a clear definition of S in a MILES code due to the absence of an explicit viscosity.

In general, the predicted turbulence variables profiles presented in figures 5 - 7 capture well the general shape of the profiles obtained by numerical simulation. But, we have to keep in mind that we are presenting a low Atwood number case. At high Atwood numbers, the variables profiles do not remain symmetrical [19]. Introduction of an asymmetry in the idealized volume fraction profiles as a function of the Atwood number might be an answer to this issue.

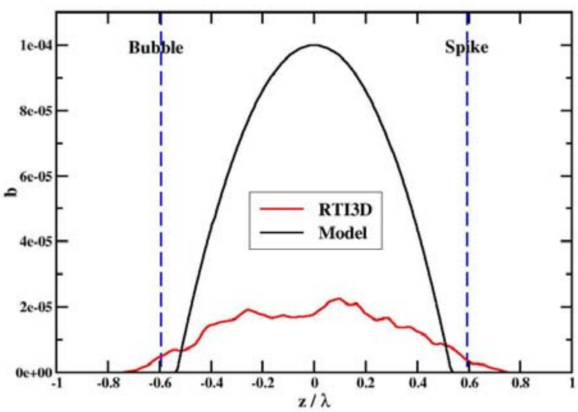

Figure 7. Density-specific volume correlation profiles in the vertical direction as predicted by the model and RTI3D simulation. Vertical dashed lines indicate bubbles and spikes fronts as predicted by RTI3D, and $\lambda = 2\pi$ is width of the computational domain**.**

CONCLUSIONS

We presented our progress toward setting initial conditions for RT simulations in the BHR turbulence model. Our approach is to provide the turbulence model with profiles of its key variables as initial conditions. These profiles present the advantage of carrying local information on the flow as well as “knowledge” of the initial conditions of the instability leading to turbulence. The determination of the turbulence variables’ initial profiles are made in 3 stages:

1. Prediction of the heights and velocities of the bubbles and spikes front using an ordinary differential equation modeling the evolution of RT instability.

2. Prediction of the fluids volume fraction profiles using a piecewise linear function between the bubbles front, the initial perturbation position and the spikes front.

3. Prediction of the turbulence model variables initial profiles using a two-fluids model and the results from steps 1 and 2.

This approach gives reasonable profiles predictions with a banded spectrum at low Atwood number.

Several points may be improved. First, the evaluation of the bubbles and spikes penetration in the case of multimode RT instability is not accurate for large Atwood numbers ($A \geq 0.4$) and does not take into account mode coupling. Second, bubbles and spikes front velocities are used in the two-fluid model formulation of the turbulence model variables in lieu of average velocity profiles of the heavy and light fluids in the mixing layer. A model for the velocity profiles would probably improve the predicted profile from a quantitative point of view. Finally, we might need to introduce more physics in the model for variable b to improve its prediction. All these points are under current investigation.

However, all the profiles shapes given by our current model are reasonable approximations. Then, the simplest way to improve the current model is to adjust the coefficients in equations $(18)-(20)$.

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