TOWARD EFFICIENT COMPUTATION OF HEAT AND MASS TRANSFER EFFECTS IN THE CONTINUUM MODEL FOR BUBBLY CAVITATING FLOWS

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Abstract

The Rayleigh-Plesset equation is used extensively to model spherical bubble dynamics, yet it has been shown that it cannot correctly capture damping effects due to mass and thermal diffusion. Full single bubble models have been successfully used to study these diffusion effects, but these are too computationally expensive to implement into the continuum model for bubbly cavitating flows since the diffusion equations must be solved in the radial direction at each position in the flow. The focus of the present research is the development of simpler and more efficient bubble dynamic models that capture the important aspects of the diffusion processes. We present some preliminary results from a full bubble model that has been developed to provide insight into possible simplifications. This in turn can be used to develop and validate simpler models. The full model is contrasted to the Rayleigh-Plesset equation, and a suggestion for possible improvement to the Rayleigh-Plesset equation is made.

1 Introduction

A model that couples the Rayleigh-Plesset equation for bubble dynamics with the continuum equations of continuity and momentum (van Wijngaarden 1968) has been used extensively in the computation of bubbly cavitating flows (Shimada et al. 1999, Wang & Brennen 1999, Colonius et al. 2000). Recently, Preston et al. (2001) employed the continuum model in the computation of cavitating flow in a converging-diverging nozzle and showed good agreement to experiments both with and without shock waves. While the model has enabled a better understanding of the physics of cavitation in many different situations, a significant limitation is the use of a polytropic approximation to account for the expansion and compression of the gas bubble interior and an effective liquid viscosity to account for damping of the bubble radial motion due to many effects including thermal and mass diffusion. The correct way to model these effects would be to solve the full set of radial equations for the conservation of mass, momentum and energy in each bubble and the surrounding liquid; however this would be a huge computation.

Matsumoto & Takemura (1994) have performed detailed computations of a single gas/vapor bubble, including thermal and mass diffusion in both the gas and liquid phases, when the surrounding pressure increases stepwise. They have shown that under these conditions significant gradients of temperature and vapor concentration are formed inside the bubble, and heat and mass transfer have a great influence on the bubble motion. While this full description of a single gas/vapor bubble has not been incorporated into the continuum model, a simplified set of equations without mass diffusion have been used in the continuum model to perform computations of shock waves in a liquid containing small bubbles of non-condensible gas (Kameda & Matsumoto 1996). In their model the full equations for conservation of mass, momentum and energy were solved for the interior of each bubble within the continuum mixture. Phase change of the liquid and mass transfer across the bubble boundary were not considered. The liquid was assumed incompressible and of constant temperature, which resulted in the interior equations being coupled to a Rayleigh-Plesset-like equation for the liquid motion. Results demonstrated that the thermal gradients inside the bubble had a significant impact on the structure of the bubbly shock.

A further simpification of the equations, which has been used to study the dynamics of single oscillating gas and vapor bubbles, is to assume constant pressure in the gaseous phase. The problem can consequently be reduced to solving only diffusion equations for the temperature and vapor concentration distribution within the bubble, coupled to a Rayleigh-Plesset type equation for the bubble motion. The boundary condition for the bubble temperature can be obtained either by assuming a constant liquid temperature, or by solving the energy diffusion equation in the liquid. Prosperetti (1991) used the former in investigating pure gas bubbles, while the latter was used by Hao & Prosperetti (1999) for bubbles of pure vapor. Kawashima et al. (2000) extended these analyses to the case of a gas/vapor bubble and found, at least in the case of oscillating bubbles, that the phase change and gas diffusion at the bubble wall interact with each other in such a way as to enhance the mass transfer at the bubble wall. However, for strongly collapsing bubbles (as may occur in flows such as the cavitating nozzle) the velocities in the gas approach the gas sound speed and the assumption of constant pressure may no longer be valid. In these situations the non-uniformity of the gas pressure can lead to additional damping of the bubble motion. Moss et al. (2000) proposed a simple modification to the gas pressure term that they incorporated as an extra damping term in the Rayleigh-Plesset equation, and which could also be incorporated into the more sophisticated models mentioned above. This would enable great efficiencies to be gained by removal of the radial continuity and momentum equations from the problem.

Of course these bubble models that compute the full set of diffusion equations assume that there is no mixing of the bubble contents which would destroy thermal and mass transfer boundary layers near the bubble interface and other thermal and concentration gradients within the bubble. This disruption could well occur when the bubble is distorted by the flow in the manner documented by Ceccio & Brennen (1991) and Kuhn de Chizelle et al. (1995). Furthermore it is well recognized that when a bubble undergoes violent collapse it normally fissions into smaller bubbles. Clearly when this fission happens there may be significant dissipation (Brennen 2001) thus altering the dynamics of the bubble. In addition this fission clearly disrupts any spherically symmetric heat and mass diffusion processes. These issues have not been adequately investigated in the past and could have a significant impact on the global dynamics of bubbly flows.

In the absence of mixing and fission models we focus here on efficient ways of incorporating the thermal and mass diffusive effects into the continuum model. For this purpose we would ideally have a bubble dynamic model that did not require the solution of the radial diffusion equations, yet still managed to capture the important behaviors associated with the diffusion processes. Storey & Szeri (2001) proposed the use of a Rayleigh-Plesset equation that is modified to enable better prediction of peak temperatures, pressures and bubble composition during the collapse of a sonoluminescence bubble. The model switches between an isothermal, variable mass process when the bubble dynamics are slow enough to allow diffusion (the growth phase), and an adiabatic, constant mass process when the bubble dynamics are too fast to allow time for diffusion (during collapse and initial rebound). The switching between the two limits is governed by monitoring the representative timescales of the bubble dynamics and the diffusion processes. Although the model is successful in obtaining more accurate estimates of peak temperature, pressure and bubble composition during the first collapse it is not able to replicate the damping of bubble rebounds associated with the diffusion processes.

In the present work, we propose to investigate efficient methods of incorporating heat and mass transfer effects for spherical bubbles. Our initial step is to build up a full (expensive) single bubble model that solves the full set of conservation equations in both the gas and liquid phases. This full model can then be used to gain insight into possible simplifications that can be used to develop simpler, more efficient models, and ultimately to verify the validity of these simpler models. Once a validated simplified model for single bubble dynamics is obtained it will be implemented into the continuum model and applied to various cavitating flows, such as the nozzle of Preston et al. (2001). In the current paper we present some preliminary computations from our full bubble model and contrast it to the computations of the simple Rayleigh-Plesset equation. Based on the preliminary results some tentative suggestions for improvement to the Rayleigh-Plesset equation are made.

2 Physical Model

In the full model we solve the conservation equations of mass, momentum and energy in both the gas and liquid phases. In the gas we assume that the perfect gas law holds for the mixture of water vapor and air, and use transport properties that are mass averages of the properties of the individual components. The liquid is assumed to be incompressible, enabling the analytical integration of the continuity and momentum equations from the bubble surface to infinity. This approach precludes the need for a non-reflecting boundary condition in order to satisfy the radiation condition at infinity. We also assume that the liquid velocity at the interface is equal to the velocity of the interface. This assumption is discussed in more detail shortly. This results in a Rayleigh-Plesset-like equation, except the pressure on the gas side of the interface is obtained from solving the full conservation equations in the gas rather then making use of the polytropic assumption.

Other interface conditions are important to the computation and are worth examining in closer detail. The mass flux of vapor per unit area into the bubble is estimated from kinetic theory as,

$$\dot{m_v}'' \quad = \quad \alpha \frac{p_{v_{sat}} - p_{vg}|_{r=R}}{\sqrt{2\pi \mathcal{R}_v T_{int}}}, \tag{1}$$

where α is the accommodation coefficient which is taken to be 0.4 following Matsumoto & Takemura (1994), $p_{v_{sat}}$ is the saturation vapor pressure, $p_{vg}|_{r=R}$ is the partial pressure of vapor at the interface, $\mathcal{R}_v$ is the perfect gas constant of the water vapor, and T_{int} is the temperature of the interface.

We also have the continuity of mass of the mixture at the interface, which yields a condition on the gas velocity,

$$u_g|_{r=R} = V - \frac{\dot{m_v}'' + \dot{m_a}''}{\rho_g|_{r=R}}, \tag{2}$$

where $V = \dot{R}$ is the interface velocity and $\dot{m_a}''$ is the mass flux of air per unit area into the bubble and is determined by the mass diffusion processes in the gas and liquid phases. A similar equation holds for the liquid velocity at the interface, but the second term is about three orders of magnitude smaller due to the liquid density replacing the gas density in the denominator. Therefore the second term is neglected relative to the first term, which results in the previously mentioned assumption that the liquid velocity at the interface is equal to the interface velocity. The validity of this assumption is examined in further detail in section 3.

The mass diffusion equations in each phase are coupled by assuming Henry's Law holds and by applying conservation of individual species at the interface which yields a balance of diffusive fluxes. The energy diffusion equations are coupled by assuming the temperatures in each phase at the interface are equal (thermal equilibrium), and by balancing heat fluxes on either side of the interface with the latent energy term associated with phase change.

A spectral method is chosen to solve the set of equations, since these have been shown to be more efficient than standard finite difference methods for the solution of these problems (Kamath & Prosperetti 1989, Storey & Szeri 1999). In particular we use a Chebychev spectral method adapted from Hao & Prosperetti (1999), who solved the thermal diffusion equations in and around a pure vapor bubble under the assumption of constant pressure within the bubble. We apply the method to the full set of equations in the gas/vapor (not employing the constant pressure assumption) and the mass and thermal diffusion equations in the liquid. To ensure there is enough spatial resolution, the number of expansion modes is increased or decreased during the computation based upon the relative amplitude of the highest mode. Storey & Szeri (2000) employed a similar spectral method, but with a different choice of expansion polynomials in the liquid phase, for the solution of the full set of equations for a gas/vapor sonoluminescence bubble. However, they neglected the diffusion of dissolved gas in the liquid phase which Kawashima et al. (2000) found could interact with the phase change at the bubble wall in such a way as to enhance the mass transfer at the bubble wall.

An explicit fourth order Runge-Kutta method is used for time marching of the equations. The method uses an adaptive time stepping technique to ensure efficiency and accuracy. Because the method is explicit the time step is primarily governed by stability limitations. These become particularly limiting during the violent bubble collapse where a large number of expansion modes (and hence large number of grid points) are required. The problem is further exasperated by the choice of the Chebychev collocation points which cluster grid points near the bubble interface. Many authors have employed implicit time marching for the liquid phase to try and overcome this limitation.

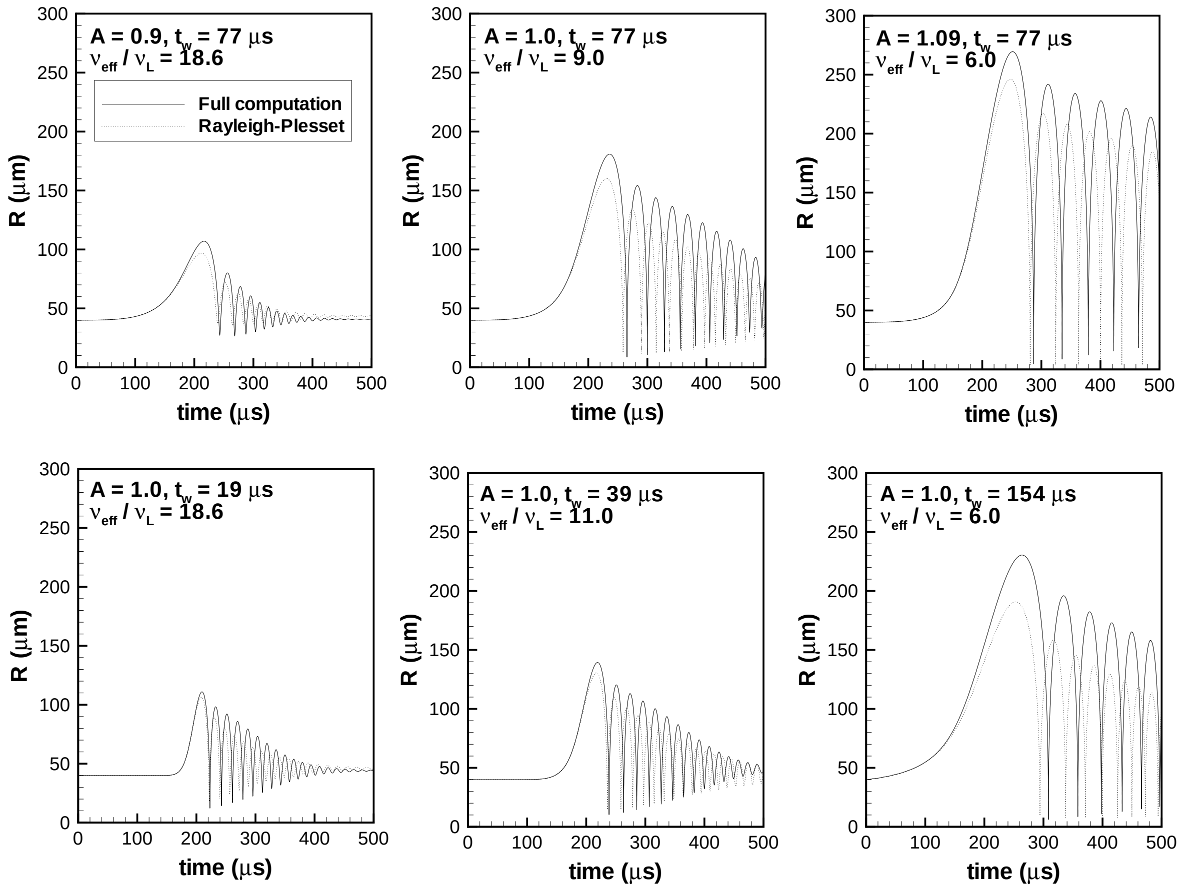

Figure 1: Comparison of full computation to Rayleigh-Plesset equation for different forcing amplitudes and durations. *Top three plots:* $A = 0.9, 1.0, 1.09$ and $t_w = 77\mu s$. *Bottom three plots:* $A = 1.0$ and $t_w = 19, 39, 154\mu s$. (The value of effective viscosity, ν_{eff}, used in the Rayleigh-Plesset equation is chosen to get a good match of the damping over the first few rebounds.)

3 Preliminary Results

In these preliminary results the effect of mass diffusion is neglected. In the application of sonoluminescence it has been shown to have minimal impact on the bubble dynamics (Storey & Szeri 1999), and the effect in the current context will be studied later. Consequently we neglect any dissolved gas in the liquid phase, and assume that the concentration of vapor in the gas phase does not vary with radial position. For initial computations the bubble is forced by a simple Gaussian pressure time history with amplitude and duration that is chosen to roughly approximate the pressure history that would be experienced by a bubble travelling through the nozzle of Preston et al. (2001);

$$p_\infty(t) = p_0 \left(1 - Ae^{-\left[\frac{t-t_0}{t_w}\right]^2}\right), \tag{3}$$

where $p_0 = 101.3kPa$ and $t_0 = 290\mu s$ in all the following computations. Figure 1 compares the current full computation with the Rayleigh-Plesset equation (RPE) for six different forcings. We see that apart from the very short duration forcings the RPE significantly underpredicts bubble growth. This is most likely to be caused by the RPE not employing the kinetic rate equation 1 for the mass flux of vapor into the bubble, resulting in an underestimate of the mass flux during the bubble expansion. In fact it is possible to use an artificially low value of the accommodation coefficient in the full computation to inhibit the mass flux of vapor

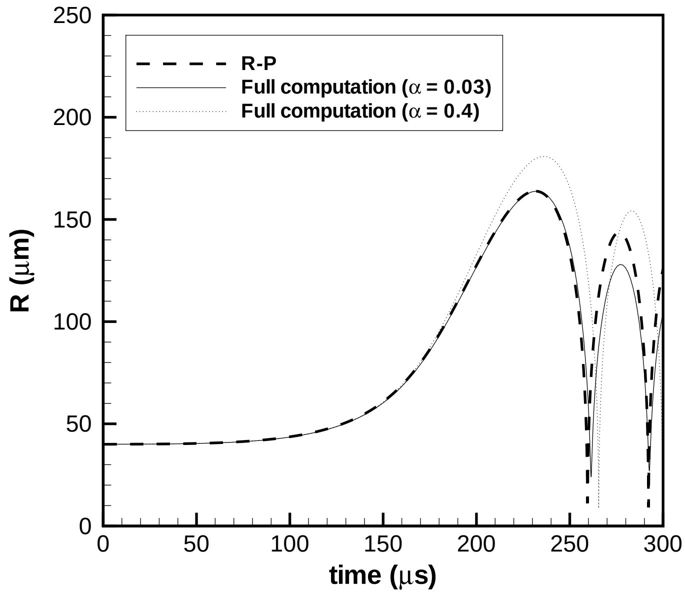

Figure 2: Comparison of full computations with different accommodation coefficients to Rayleigh-Plesset equation ($A = 1.0$ and $t_w = 77\mu s$).

and obtain good agreement with the RPE. Figure 2 shows such a computation, where the accommodation coefficient has been reduced from 0.4 to 0.03 to obtain a good match in initial bubble growth. This result immediately leads to the speculation that the RPE could be improved by the incorporation of equation 1 into the formulation, with very little computational cost. However, we must remember that the current full computation neglects any mass diffusion of vapor in the bubble which may be very important in determining the vapor pressure that appears in equation 1. Therefore this speculation needs to be revisited once the mass diffusion equations are included in the model.

Figure 2 also shows the poor ability of the RPE equation to correctly model the diffusive damping of the bubble rebounds. Improvements can be made by the use of an effective viscosity, as is done in figure 1. However, the most appropriate value of effective viscosity that should be used varies depending upon the forcing amplitude and duration and is not able to be determined without comparison to the full computation. In addition it appears that a value that is chosen to get a good match of damping over the first few rebounds fails to get a good match later in the collapse sequence. This is apparent in figure 1 where the attenuation of the first few rebounds is matched by the RPE, but is then underpredicted by the RPE over the later rebounds. The limitations of the use of effective viscosity to account for thermal damping in the non-linear oscillations of bubbles has been well documented (Prosperetti et al. 1988, Prosperetti 1991). In application to the continuum model these limitations would have significant impact on the structure of a bubbly shock as discussed by Kameda & Matsumoto (1996).

With the current model we are able to examine the validity of the assumption that the liquid velocity at the interface is approximately equal to the velocity of the interface itself. Hao & Prosperetti (1999) have made an order of magnitude analysis that shows that additional velocities due to phase change at the interface are about three orders of magnitude smaller than the typical interface velocities, and can therefore be ignored. However, if there is substantial velocity due to phase change at instances where the interface velocity is near zero (top of expansion phase and rebounds, and instantaneously during collapse) then this order of magnitude analysis may not hold. Figure 3 plots the interface velocity, and the additional velocities in the gas and liquid phases due to phase change at the interface for a typical computation. The additional gas velocity is simply the last term of equation 2 with $\dot{m}''_a = 0$ and is included in the computation, while the addtional liquid velocity is obtained by replacing the gas density with the liquid density, and is neglected in

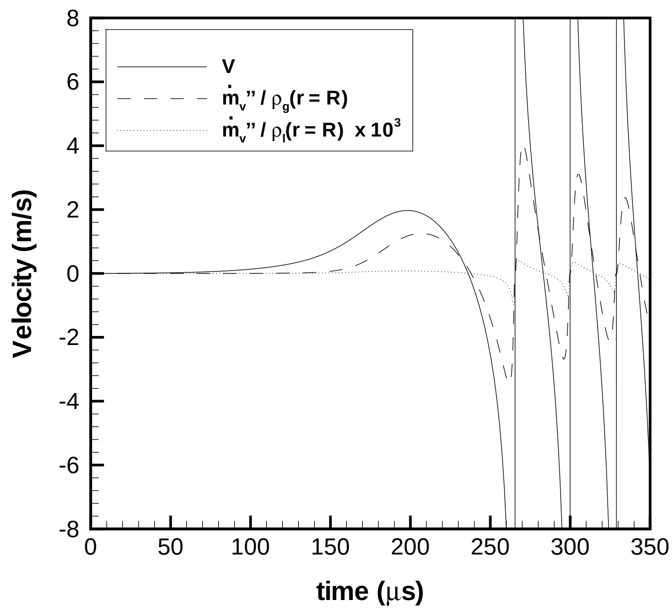

Figure 3: Interface velocity, V, additional velocity in gas due to phase change, $\dot{m}_v''/\rho_g|_{r=R}$, and additional velocity in liquid due to phase change, $\dot{m}_v''/\rho_l|_{r=R}$, for a typical full computation ($A = 1.0$ and $t_w = 77\mu s$).

the computation. We see that the additional liquid velocity is at least three orders of magnitude smaller than the interface velocity. Closer study of the plot also indicates that when the interface velocity is approximately zero the additional liquid velocity is also zero and hence it can be neglected for the entire computation. On the other hand, the additional gas velocity is often of the same order as the interface velocity and must be included in the computation.

4 Conclusions

A single bubble model that solves the full set of conservation equations in both the gas and liquid phases of a spherical bubble has been developed for the purpose of validating simpler bubble dynamic models. Preliminary results contrast the damping behaviors of the full model with the standard Rayleigh-Plesset equation, and also suggest some scope for immediate improvement of the Rayleigh-Plesset equation by the incorporation of a rate equation for evaporation and condensation at the interface. The full model has also been used to validate the commonly used assumption that the liquid velocity at the interface is approximately equal to the interface velocity, while showing that a similar assumption on the gas velocity is not valid. Future work will focus on using the full model in the development of simpler more efficent bubble dynamic models that still capture the important aspects of the diffusion processes. These models will then be implemented into the continuum model and applied to various cavitating flows.

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