Numerical Simulation of Nonlinear Acoustic Waves in Two-Phase Fluid

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Abstract

Nonlinear acoustic wave propagation equation with void fraction (volume fraction of gas phase) is derived and numerically solved for the simulation of HIFU (High Intensity Focused Ultrasound) with micorbubbles in the present paper. HIFU is one of promising treatments for cancer. The focused pressure waves generate heat and necrose cancer cells. It has been lately reported that the existence of micorbubbles enhances heating at the focal area and the present paper is intended to clarify this mechanism with numerical approach. After describing the derivation of the governing equations and the detail of the numerical method, computed results with varying initial void fractions and bubble sizes are presented to show the propagation of ultrasound and the bubble motions in the focal area. Additionally heat generation by microbubbles are also simulated and evaluated.

Keywords: Ultrasound, Bubble, CFD, Multiphase, HIFU (High Intensity Focused Ultrasound)

Introduction

HIFU (High Intensity Focused Ultrasound) is a promising treatment for cancer because of its low invasiveness, high controllability and low cost compared with other existing methods. On the other hand, HIFU has a problem when it is applied to deep body such as liver cancer. Ultrasound may reflect and refract due to non-uniformity of body tissue and the focal area then shifts or diffuses. At the same time, attenuation of ultrasound during the propagation is not also negligible. As a result, insufficient energy reaches the lesion. To overcome this problem, utilization of microbubbles is proposed (Bailey et al., 2001; Holt and Roy, 2001). Bubbles exposed in ultrasound oscillate volumetrically and convert kinetic energy of ultrasound into heat energy. This phenomenon has been experimentally observed but the detailed mechanism has not yet been clear. In this paper, ultrasound wave propagation in fluid with microbubbles is numerically simulated. First, nonlinear acoustic wave propagation equation with void fraction (volume fraction of gas phase) is derived. Second, the above equation is solved with Keller equation that describes the volumetric motion of a bubble, varying initial bubble size and void fraction. Finally heat generation by bubbles is numerically simulated solving the heat conduction equation to evaluate the effect of bubbles.

Derivation of Equations

Nonlinear acoustic wave propagation equation with void fraction is derived from the following two conservation equations and one constraint.

• *Conservation of mass*

$$\frac{\partial(f_L \rho_L)}{\partial t} + \frac{\partial(f_L \rho_L u_{Lj})}{\partial x_j} = 0 \tag{1}$$

• *Conservation of momentum*

$$\frac{\partial\left(f_L\rho_L u_{Li}\right)}{\partial t}+\frac{\partial\left(f_L\rho_L u_{Li}u_{Lj}\right)}{\partial x_j}=-\nabla_i P \tag{2}$$

• *Volume constraint*

$$f_G+f_L=\frac{4}{3}\pi r_G^3 n_G+f_L=1 \tag{3}$$

Suffix L denotes liquid and G denotes gas. f the volume fraction, ρ the density, u the velocity, P the pressure and r the radius. Here bubbles are assumed to be all spherical and to keep number density n_G be constant. Following the derivation of KZK (Khokhlov – Zabolatskaya – Kuznetsov) equation (Zabolotskaya and Khokhlov, 1969; Kuznetsov, 1970) to introduce small perturbation up to the second order terms and Aubry et al.'s idea of ultrasound propagation in inhomogeneous medium (Aubry et al., 2003), the following equation is obtained finally.

$$\begin{aligned}\frac{\partial^2(f_L p)}{\partial t^2}&=c_{L0}^2\left(2\frac{\partial^2 p}{\partial x_j^2}-\frac{\partial}{\partial x_j}\left(f_L\frac{\partial p}{\partial x_j}\right)\right)+\frac{\beta}{\rho_{L0}c_{L0}^2}\frac{\partial^2}{\partial t^2}\left(f_L p^2\right)\\&+\frac{\lambda_L}{\rho_{L0}c_{L0}^2}\left(\frac{1}{c_{vL}}-\frac{1}{c_{pL}}\right)\frac{\partial^2}{\partial t^2}\left(f_L\frac{\partial p}{\partial t}\right)+\frac{\partial}{\partial t}\left(p\frac{\partial f_L}{\partial t}\right)-\rho_{L0}c_{L0}^2\frac{\partial^2 f_L}{\partial t^2}\end{aligned} \tag{4}$$

where λ is heat conductivity, c is speed of sound, p is perturbation pressure, c_v and c_p are specific heat at constant volume or pressure, respectively and suffix 0 denotes the equilibrium state. β is called nonlinear coefficient and is a material property. For volumetric oscillation of bubbles, the Keller's equation (Keller and Kolodner, 1956) is solved together with eq. (4).

$$\begin{aligned}&r_G\left(1-\frac{1}{c_{L0}}\frac{dr_G}{dt}\right)\frac{d^2 r_G}{dt^2}+\frac{3}{2}\left(1-\frac{1}{3c_{L0}}\frac{dr_G}{dt}\right)\left(\frac{dr_G}{dt}\right)^2\\&=\frac{1}{\rho_{L0}}\left(1+\frac{1}{c_{L0}}\frac{dr_G}{dt}+\frac{1}{c_{L0}}r_G\frac{d}{dt}\right)\left(P_G-\frac{2\sigma}{r_G}-\frac{4\mu_L}{r_G}\frac{dr_G}{dt}-P_L\right)\end{aligned} \tag{5}$$

where r_G is bubble radius, σ is the surface tension, μ is viscosity coefficient. P_G, the pressure inside of the bubble, is obtained with a reduced-order model (Preston and et al., 2002; Sugiyama et al., 2005). Lastly the heat conduction equation (6) is used for estimating the temperature rise around the focal area.

$$\rho_L c_{pL}\frac{\partial T}{\partial \tau}=\frac{\partial}{\partial x}\left(\lambda_L\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial r}\left(\lambda_L\frac{\partial T}{\partial r}\right)+\frac{1}{r}\left(\lambda_L\frac{\partial T}{\partial x}\right)+\overline{W}_{th}+\overline{W}_{vis} \tag{6}$$

where $\overline{W}_{th}$ and $\overline{W}_{vis}$ are time-averaged heat source terms of

$$\begin{aligned}W_{th}&=-\lambda_G\left.\frac{\partial T}{\partial r}\right|_{r=R}\cdot 4\pi r_G^2\\W_{vis}&=4\mu_L\frac{1}{r_G}\frac{dr_G}{dt}\frac{dr_G}{dt}\cdot 4\pi r_G^2\end{aligned} \tag{7}$$

and they are the thermal conduction from a bubble and the viscous dissipation of surrounding liquid, respectively.

Numerical Methods

Equations (4) and (6) are solved by a finite difference method. The spatial terms are discretized with second order central difference and the temporal terms are discretized with second order backward difference, resulting the second order accuracy scheme. The Keller's equation (5) is integrated with 2nd order Runge-Kutta method.

Results and Discussions

The present problem setup is illustrated in Fig. 1. The right hand side of area is assumed to be human body and bubbles are uniformly distributed. The outside of the body is filled with water. Thus reflection and fraction are expected to occur at the interface. Typical conditions are summarized in Table 1.

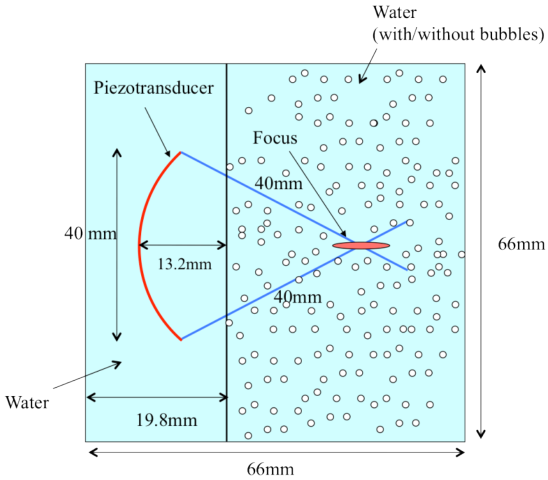


Figure 1. Problem Setup

Table 1. Summary of conditions

Liquid phase, Gas phase	Water, Air
Liquid density	1,000 kg/m^3
Sound speed of liquid	1,500 m/s
Liquid viscosity	8.64×10^{-4} Pa·s
Liquid specific heat at constant pressure	4.179 J/kg K
Liquid specific heat ratio	1.012
Liquid thermal conductivity	6.1×10^{-1} W/m K
Coefficient of nonlinearity	3.5
Initial pressure	101.3 kPa
Input frequency	1.0 MHz
Wave cycle	Continuous wave
Void fraction	0.0, 1.0×10^{-6}, 10^{-5}, 10^{-4}
Bubble radius	2.4, 3.4, 4.4, 10.0 μm
Surface tension	7.2×10^{-2} N/m
Gas specific heat ratio	1.4

First, Figure 2 shows a comparison with the other research result (Okita et al., 2012) of similar problem setting, solved with a stricter but more time consuming method. The maximum pressure distribution on the axis of symmetry shows good agreement, especially the pressure drop at the focal area with higher void fraction case. Figures 3 show maximum absolute pressure distribution under the continuous wave radiation with two void fractions. High void fraction prevents ultrasound to penetrate and the pressure in focal area is much lower. Figures 4 compare the effect of bubble size with initial void fraction of 10^{-6}. The radius of 3.4μm is the resonance radius of 1MHz for the linear theory. However the result suggests that 2.4μm is closer to the resonance due to the nonlinear effect, because the bubbles react more violently.

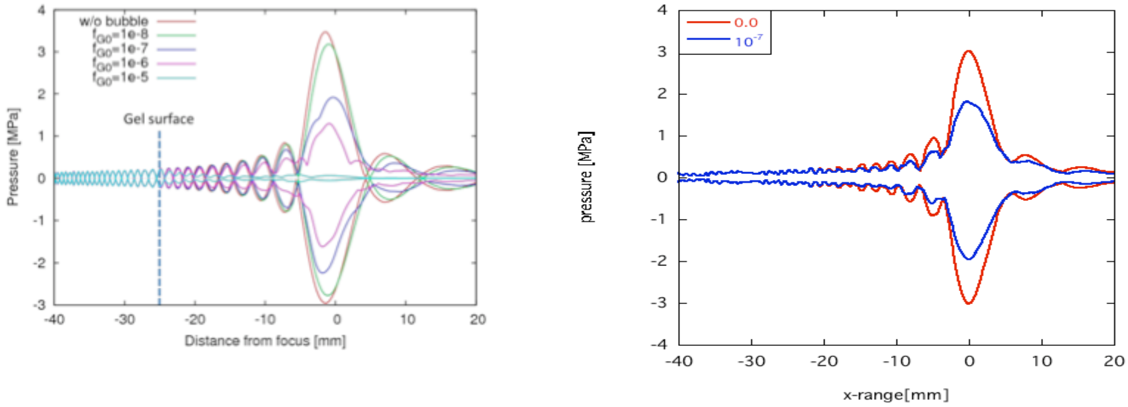
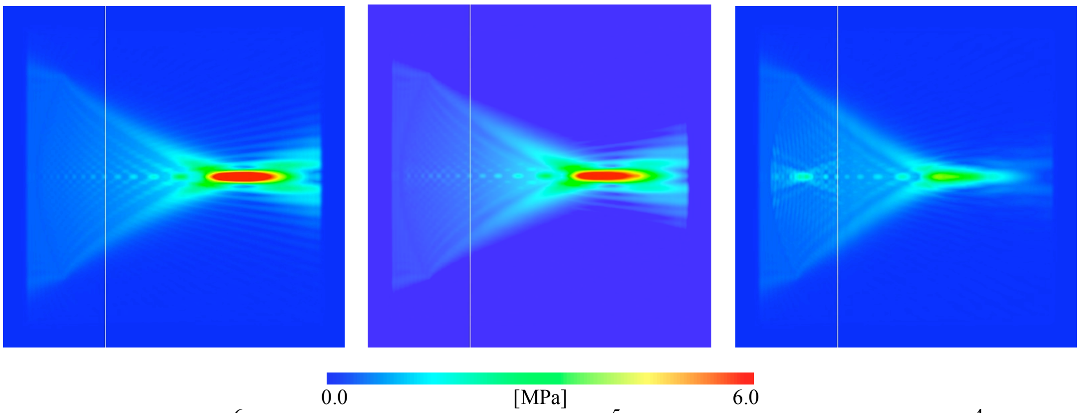
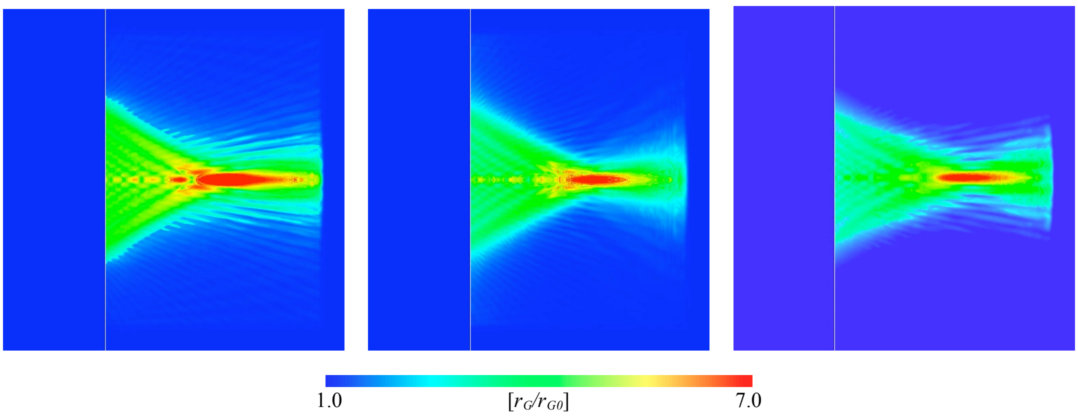


Figure 2 Validation of the present method; maximum pressure distribution on the axis of symmetry. left: Okita et al. (2012), right: present



(a) $f_{G0}=10^{-6}$ (b) $f_{G0}=10^{-5}$ (c) $f_{G0}=10^{-4}$

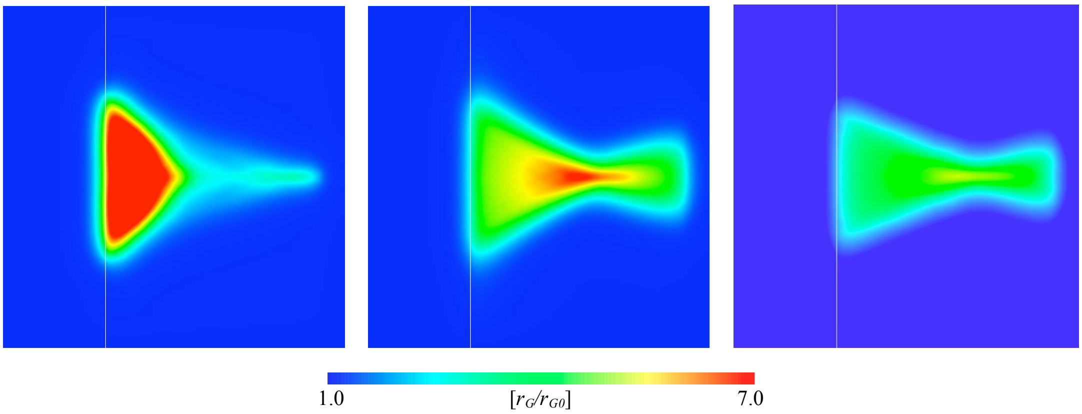
Figure 3 Pressure distribution for different void fractions



(a) r_{G0}=2.4[μm] (b) r_{G0}=3.4[μm] (c) r_{G0}=4.4[μm]

Figure 4 Maximum radius distribution for different initial radius

Finally, Figures 5 give temperature rise due to the bubbles after 30 second in cases of Fig. 3. In the case of 2.4μm radius, bubbles oscillate close to the interface and thus the temperature at the focal area does not rise.



(a) r_{G0}=2.4[μm] (b) r_{G0}=3.4[μm] (c) r_{G0}=4.4[μm]

Figure 5 Temperature rise for different initial radius

Conclusions

In order to be applied for HIFU simulation, nonlinear acoustic wave propagation equation with void fraction was derived and numerically solved with Keller's equation. A simple setup of focused ultrasound field with microbubbles gave reasonable results and revealed the effect of void fraction and bubble size. Heat conduction equation was also solved to demonstrate the heat generation of bubbles.

Acknowledgments

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