Computations of Compressible Two-phase Flow using Accurate and Efficient Numerical Schemes

Chongam Kim *

* Department of Aerospace Engineering, Seoul National University, Seoul, Korea
Tel : +82-2-880-1915; E-mail: chongam@snu.ac.kr

Abstract: RoeM and AUSMPW+ schemes are two of the most accurate and efficient schemes which are recently developed for the analysis of single phase gas dynamics. In this paper, we developed two-phase versions of these schemes for the analysis of gas-liquid large density ratio two-phase flow. We adopt homogeneous equilibrium model (HEM) using mass fraction to describe different two phases. In the Eulerian-Eulerian framework, HEM assumes dynamic and thermal equilibrium of the two phases in the same computational mesh. From the mixture equation of state (EOS), we derived new shock-discontinuity sensing term (SDST), which is commonly used in RoeM and AUSMPW+ for the stable numerical flux calculation. The proposed two-phase versions of RoeM and AUSMPW+ schemes are applied on several air-water two-phase test problems. In spite of the large discrepancy of material properties such as density, enthalpy, and speed of sound, the numerical results show that both schemes provide very satisfactory solutions.

Keywords: two-phase flow, RoeM scheme, AUSMPW+ scheme, shock discontinuity sensing term

1. INTRODUCTION

Due to its large application areas involving hydraulic machine, underwater high-speed vehicle, liquid fuel rocket, etc., the computation of compressible multiphase flows has received a growing attention in recent years. We are interested in the accurate and robust simulation of gas-liquid two-phase flows with compressibility effect. Among the numerous levels of physical multiphase modeling, homogeneous equilibrium model (HEM) using mass fraction is adopted in this paper.

For the high resolution simulation, we developed the two-phase versions of RoeM [1] and AUSMPW+ [2] schemes which are originally developed for the high resolution simulation of high-speed gas dynamics. The RoeM scheme, based on Roe's flux difference splitting (FDS), is a shock-stable scheme without any tunable parameters while maintaining the accuracy of the original Roe scheme. The AUSMPW+ scheme is the improved version of AUSMPW scheme. By the use of pressure based weighting functions, AUSMPW+ can reflect both properties of a cell interface adequately, and its numerical results show the successful elimination of oscillations and overshoots behind shocks and near a wall. Both RoeM and AUSMPW+ schemes are among recently developed advanced schemes for the gas dynamics. The purpose of this paper is to extend both schemes to two-phase flows without losing their original ideas and merits.

Difficulties in extending RoeM and AUSMPW+ to two-phase flows are not far different from those in general two-phase calculation. One lies in the treatment of the equation of state (EOS). The definition of mixture density plays the role of mixture EOS in HEM. From the mixture EOS, we introduce new pressure weighting terms, which are commonly used in RoeM and AUSMPW+ to sense the shock discontinuity. The other difficulty is the fluxes at the phase interface. Due to the advection property of AUSM-type scheme, the original AUSMPW+ could cause numerical instability near the large density ratio phase interface. To overcome this instability problem, we scale the control function *f* instead of using non-conservative approaches such as ghost fluid method.

The present paper organized as follows. After introduction, governing equations with the EOS for each phase is given. In section 3, new shock discontinuity sensing term is introduced and two phase versions of the RoeM and AUSMPW+ schemes are presented in section 4 and 5. Numerical results for well known test problems are appeared in section 5. Finally, conclusion is given in section 6.

2. GOVERNING EQUATIONS

HEM [3] with mass fraction is adopted to describe two-phase flows. As we assumed fully compressible flows, the governing equations are consisted of mixture mass, momentum, and energy conservation laws together with one phase mass conservation law. The two-dimensional Euler equations are as follows:

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}=0, \qquad (1)$$

where Q is the state vector, and E and F are flux vectors.

For compressible two-phase flows with mass fraction, the state and flux vectors have the form:

$$Q=[\rho_m,\rho_m u,\rho_m v,\rho_m E_t,\rho_m Y_1]^T, \qquad (2)$$

$$E=[\rho_m U,\rho_m uU+n_x p,\rho_m vU+n_y p,\rho_m HU,\rho_m Y_1 U]^T. \qquad (3)$$

Contra-variant velocity $U=n_x u+n_y v$ means control surface-normal velocity component. And Y_1 stands for the mass fraction of gas phase.

The following definition of mixture density, ρ_m, has the role of mixture EOS [4] combined with each phase's EOS:

$$\rho_m=\frac{1}{\sum_i \frac{Y_i}{\hat{\rho}_i(p,T)}}=\frac{1}{\sum_i \frac{Y_i}{\hat{\rho}_i(p,h_i)}} \qquad (4)$$

In Eq. (4), $\hat{\rho}_i$ means density defined on the occupied volume of i-th fluid, while ρ_m is defined on the each control volume (or each computational mesh).

We adopted 'the EOS for stiffened fluid' for liquid phase, which has the following form [5]:

$$p=(n-1)\rho e-np_c, \qquad (5)$$

where $n=7.0$, $p_c=3.03975\times10^8$ Pa.

And ideal gas EOS is used for gas phase:

$$p=(\gamma-1)\rho e, \qquad (6)$$

where $\gamma=1.4$.

At atmospheric pressure ($p = 101325.0$ Pa), the density of liquid comes to $\rho = 1000.0$ kg/m^3, and the density of gas becomes $\rho = 1.225$ kg/m^3.

From the following assumption of dynamic and thermal equilibrium, the total system is closed:

$$p = p_l = p_g \,,\; T = T_l = T_g . \qquad (7)$$

3. SHOCK DISCONTINUITY SENSING TERM

The pressure ratio term " $\min(\frac{p_L}{p_R}, \frac{p_R}{p_L})$ " at the control surface (i.e., computational cell interface) is used both in RoeM and AUMSPW+ to sense the shock discontinuity and control the proper numerical fluxes. For the single phase flows of gas dynamics, the direct use of real pressure ratio works well. In the liquid phase, however, due to the large density and high speed of sound, pressure field varies drastically even for non-shock region. This means that our schemes could lose their accuracy near liquid region. So the proper scaling of the shock discontinuity sensing term is required.

Development of a new SDST is a scaling problem near liquid phase. The main idea of the scaling starts from the derivation process of the AUMSPW scheme [6]. At first, through the analysis of AUSM+ and AUSMD, density ratio was chosen to determine the consideration of physical properties on both sides. And, after assuming the interfacial common speed of sound, the density ratio was changed into the pressure ratio.

In the same manner, we start from the density ratio, and try to change it into the pressure ratio. With the mixture EOS applied to the speed of sound, the density is given by

$$\rho_m = \frac{\dfrac{\partial \rho_m}{\partial p}}{\dfrac{\alpha_1}{\gamma p} + \dfrac{1-\alpha_1}{n(p+p_c)}} , \qquad (8)$$

where ρ_m is a mixture density, c_m is a mixture speed of sound, α_1 is a volume fraction of gas phase, and γ, n, p_c are constant coefficients from the EOS.

If we assume to use the interfacial common $\partial \rho_m / \partial p$ and volume fraction, we can define following pressure function $\bar{p}_{L,R}$:

$$\bar{p}_{L,R} = \frac{1}{\dfrac{\alpha_1}{\gamma p_{L,R}} + \dfrac{1-\alpha_1}{n(p_{L,R}+p_c)}} . \qquad (9)$$

Then, density ratio can be changed into pressure ratio:

$$\frac{\rho_{m,L}}{\rho_{m,R}} \approx \frac{\bar{p}_L}{\bar{p}_R} . \qquad (10)$$

Now we can use " $\min(\frac{\bar{p}_L}{\bar{p}_R}, \frac{\bar{p}_R}{\bar{p}_L})$ " as a shock discontinuity sensing term. In order to validate the developed SDST for two-phase flow, the proposed pressure function's ratio $\bar{p}_R / \bar{p}_L$ is checked on 1-D mixture shock relation. As we can see in Table 1, the scaled pressure ratio $\min(\frac{\bar{p}_L}{\bar{p}_R}, \frac{\bar{p}_R}{\bar{p}_L})$ has the value of about 1/O(1) even for the near liquid phase. So we can expect that our new SDST will not work on smooth region even in near liquid phase.

Here, we want to mention that we can use the same SDST form for all mixture flows regardless of mass fraction, mixture density, and mixture speed of sound. And we also mention that the same SDST form can be derived for isothermal two-phase flows, too, if we use stiffened fluid type EOS for liquid phase.

4. ROEM SCHEME FOR TWO-PHASE FLOW

In the compressible two-phase flow, direct derivation of the system Jacobian matrix using conservative variables is very hard due to its complicated form of EOS. Moreover, due to the large speed of sound at liquid phase, many two-phase flow analyses require preconditioning technique, which alters the governing system to primitive variable-based form. So the Roe scheme based on primitive variables are popularly used instead of the original conservative variable based Roe scheme in the two-phase flow research area. The primitive variable

Table 1 Magnitude of pressure ratio and developed function's ratio on 1-D shock relation

p_L=101325Pa	c_L (m/s)	ρ_L (kg/m^3)	M_L=1.5		M_L=2.0	
Mass fraction			p_R / p_L	$\bar{p}_R / \bar{p}_L$	p_R / p_L	$\bar{p}_R / \bar{p}_L$
Y_1=0.0 (pure liquid)	1458.95	1000.00	6565.685	3.18750	15756.3	6.25000
$Y_1=1.0\times10^{-8}$	1347.99	999.99	4836.944	2.61162	12682.5	5.22595
$Y_1=1.0\times10^{-7}$	885.63	999.92	8.24318	1.22860	2494.80	1.83307
$Y_1=1.0\times10^{-6}$	342.81	999.19	2.42609	2.06508	4.84434	2.78550
$Y_1=1.0\times10^{-5}$	112.01	991.91	2.26608	2.22898	4.06936	3.83132
$Y_1=1.0\times10^{-4}$	38.10	924.61	2.25124	2.24752	4.00529	3.98094
$Y_1=1.0\times10^{-3}$	20.23	550.87	2.24981	2.24943	3.99909	3.99665
$Y_1=1.0\times10^{-2}$	32.26	109.25	2.25005	2.25001	3.99940	3.99915
$Y_1=1.0\times10^{-1}$	92.31	12.12	2.25426	2.25426	4.00948	4.00946
Y_1=1.0 (pure gas)	340.29	1.225	2.45833	2.45833	4.50000	4.50000

based Roe scheme in our two-phase model can be summarized as follows:

$$
\begin{aligned}
E_{1/2} &= \frac{1}{2}(E_L + E_R - \Gamma_{e,1/2} \,|\, \Gamma_e^{-1} A_p \,|_{1/2}\, \Delta Q_p) \\
&= \frac{1}{2}(E_L + E_R - \Gamma_{e,1/2} \,|\, \tilde{A}(Q_L, Q_R) \,|_{1/2}\, \Delta Q_p), \\
&= \frac{1}{2}(E_L + E_R - \Gamma_{e,1/2} X \,|\, \Lambda \,|\, X^{-1} \Delta Q_p)
\end{aligned}
\qquad (11)
$$

where $\Gamma_e = \dfrac{\partial Q}{\partial Q_p}$ and $A_p = \dfrac{\partial E}{\partial Q_p}$.

And our choice of primitive variables is

$$Q_p = [p, u, v, h_m, Y_1]^T. \qquad (12)$$

After grouping subsonic numerical dissipation parts by two common eigenvalues, Roe scheme can be converted into HLLE-like form. And by introducing control functions *f* and *g*, the RoeM scheme for compressible two-phase flow is derived and summarized as follows:

$$
\begin{aligned}
E_{1/2} = \frac{1}{2}[E_L + E_R - \tilde{M} A_p \Delta Q_p \\
+ \hat{c}(\tilde{M}^2 - 1)\Gamma_e \Delta Q_p + g\hat{c}(1 - |\tilde{M}|) B\Delta Q]
\end{aligned}
, \qquad (13)
$$

$$
B\Delta Q = (\Delta\rho_m - f\frac{\Delta p}{\hat{c}_m^2})\begin{pmatrix} 1 \\ \hat{u} \\ \hat{v} \\ \hat{H} \\ \hat{Y}_1 \end{pmatrix} + \hat{\rho}_m \begin{pmatrix} 0 \\ \Delta u - n_x \Delta U \\ \Delta v - n_y \Delta U \\ \Delta H - \hat{U}\Delta U - \dfrac{\Delta p}{\hat{\rho}_m} \\ \Delta Y_1 \end{pmatrix},
$$

$$
f = \begin{cases} 1 & , \hat{u}^2 + \hat{v}^2 = 0 \\ |\hat{M}|^h & , \hat{u}^2 + \hat{v}^2 \neq 0 \end{cases},
$$

$$h = 1 - \min(P_{i+1/2,j}, P_{i-1/2,j}, P_{i,j+1/2}, P_{i,j-1/2}),$$

$$P_{i+1/2,j} = \min\left(\frac{\bar{p}_{i,j}}{\bar{p}_{i+1,j}}, \frac{\bar{p}_{i+1,j}}{\bar{p}_{i,j}}\right),$$

$$
g = \begin{cases} |\hat{M}|^{1-\min\left(\frac{\bar{p}_{i,j}}{\bar{p}_{i+1,j}}, \frac{\bar{p}_{i+1,j}}{\bar{p}_{i,j}}\right)} & , \hat{M} \neq 0 \\ 1 & , \hat{M} = 0 \end{cases},
$$

where $\hat{M} = \dfrac{\hat{U}}{\hat{c}}$.

The properties with hat symbol indicate Roe average values. $B\Delta Q$ term does not exist in HLLE scheme, and RoeM controls this part near the shock discontinuity.

It is noted that Mach number-based functions *f* and *g* are introduced to balance damping and feeding rates, which leads to a shock-stable Roe scheme. And the new SDST is used in both *f* and *g*.

5. AUSMPW+ SCHEME FOR TWO-PHASE FLOW

Contrary to FDS type schemes, AUSM type schemes have an advantage in the application to complicated fluid systems, because a consistent vector form used in single phase can be extended. In the following, the AUSMPW+ scheme for the two-phase flow is given.

$$E_{1/2} = \bar{M}_L^+ c_{1/2}\phi_L + \bar{M}_R^- c_{1/2}\phi_R + (P_L^+ p_L + P_R^- p_R), \qquad (14)$$

1) $M_{1/2} \geq 0$

$$\bar{M}_L^+ = M_L^+ + M_R^-[(1-\omega)(1+f_R) - f_L],$$

$$\bar{M}_R^- = M_R^- \omega (1 + f_R)$$

2) $M_{1/2} < 0$

$$\bar{M}_L^+ = M_L^+ \omega (1 + f_L),$$

$$\bar{M}_R^- = M_R^- + M_L^+[(1-\omega)(1+f_L) - f_R]$$

where $\omega = \max(\omega_1, \omega_2)$,

$$\omega_1 = 1 - \min\left(\frac{\bar{p}_L}{\bar{p}_R}, \frac{\bar{p}_R}{\bar{p}_L}\right)^3,$$

$$\omega_2 = 1 - \frac{\min(\bar{p}_{1,L}, \bar{p}_{1,R}, \bar{p}_{2,L}, \bar{p}_{2,R})}{\max(\bar{p}_{1,L}, \bar{p}_{1,R}, \bar{p}_{2,L}, \bar{p}_{2,R})},$$

$$f_{L,R} = \left(\frac{\bar{p}_{L,R}}{\bar{p}_s} - 1\right) \times (1 - \omega_2) \times \min\left(\frac{\rho_{m,L}}{\rho_{m,R}}, \frac{\rho_{m,R}}{\rho_{m,L}}\right),$$

$$\phi = (\rho_m, \rho_m u, \rho_m v, \rho_m H, \rho_m Y_1)^T.$$

Note that the speed of sound at phase interface is lower than that of either phases, because HEM allows mixture region. From the mixture EOS, typical averaging of mass fraction at phase interface can reflect this characteristic, but any averaging of left and right speed of sound cannot predict this low speed of sound. Among the several candidates, we use Roe type speed of sound in the numerical tests.

It is noted that AUSMPW+ can reflect the flux by pressure difference with the help of control function *f*. In two-phase flows, however, if pressure difference coinsides with large density ratio phase interface, the flux by pressure difference could be too large, because of the advection property of AUSM-type schemes, causing numerical instabilities. So, in order to stabilize the scheme near the large density ratio phase interface, we modified the function *f* by considering density ratio of both sides.

Our modifications for two-phase version AUSMPW+ scheme can be summarized as follows.

- M1: Introduction of new SDST
- M2: Use of Roe type speed of sound at the control surface
- M3: Modification of function *f* to consider the density ratio of both sides

6. NUMERICAL RESULTS

6.1 Odd-Even Decoupling Test

In order to test the shock stability of the schemes, we solved two-phase mixture moving shock problem on a perturbed grid. In this “Quirk’s test,” it is known that the schemes which cause shock instability phenomenon destroy the original moving shock profile by amplifying the numerical errors coming from the perturbed grid system. In gas dynamics, RoeM and AUSMPW+ show shock-stable characters while the original Roe scheme provides solution with numerical errors.

Fig. 1 shows the results of each scheme for $Y_1 = 0.1$ mixture flow. While Roe scheme destroys the normal shock structure, both RoeM and AUSMPW+ clearly capture the shock, showing their robust and stable behavior even in the two-phase flow region.

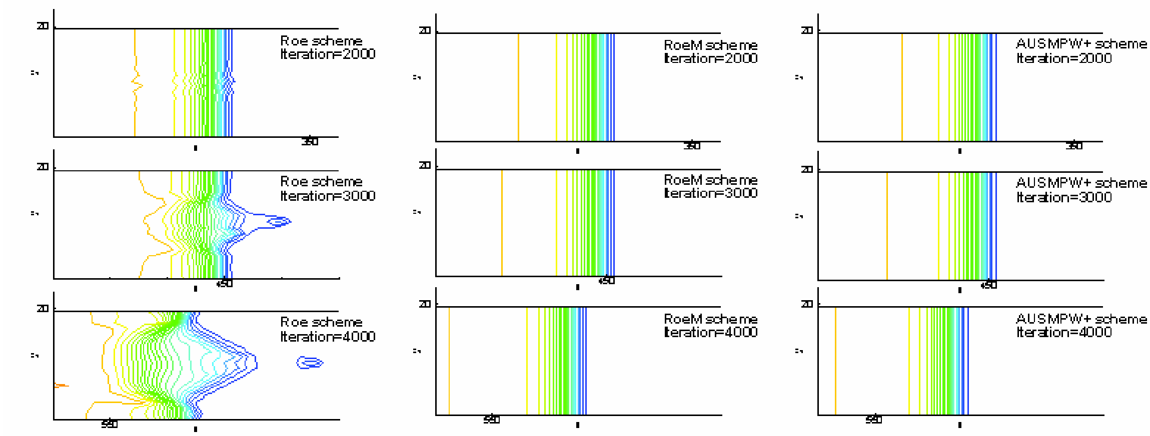

Fig. 1 Quirk's test on Y_1 = 0.1 mixture flow(density contour)

6.2 Liquid Shock-Phase Interface Interaction (SII)

In this challenging problem, the liquid shock of M=1.7 encounters with the phase interface of about 1:1000 density ratio. Initial right-going liquid shock is located at x=0.1, and the phase interface is at x=0.5. Results at t=0.3ms are shown in Fig. 2~4. Well known physics including shock transmission/reflection pattern, generation of constant velocity region after the shock-phase interface interaction are shown. (line: initial, circle: RoeM, filled square: AUSMPW+)

When the liquid shock interacts with phase interface, reflection wave is a rarefaction wave, while incident wave is still a shock wave. In Fig. 2, the incident shock wave in gas is located at x=0.65, and the end of rarefaction wave is located at x=0.42. This can be noticed from Fig. 4. Both liquid and gas phases are moving at the same velocity in the region x=[0.42, 0.65] after the shock-interface interaction. It is noticed that both RoeM and AUSMPW+ with the modified SDST work well in this simulation in spite of large density and pressure ratio.

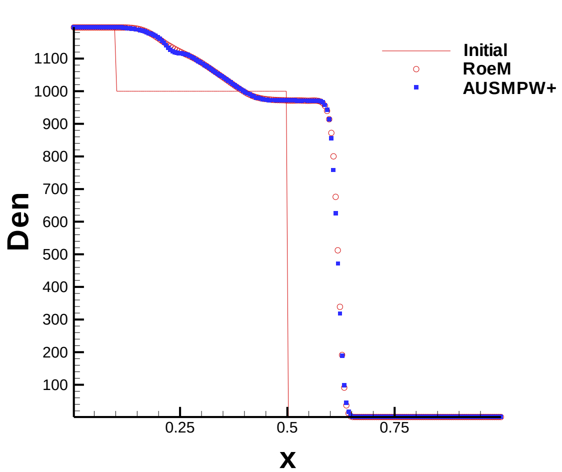

Fig. 2 Density distribution at t=3×10^{-4}

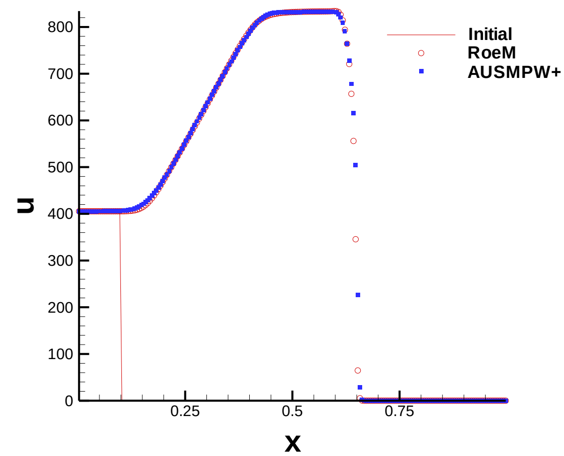

Fig. 3 Velocity distribution at t=3×10^{-4}

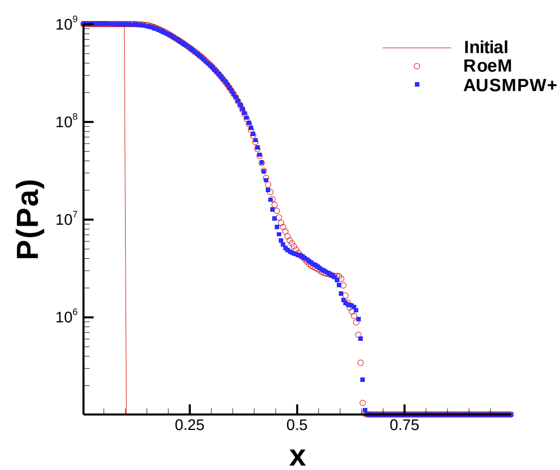

Fig. 4 Pressure distribution at t=3×10^{-4} (log scale)

6.3 2-D Shock-Bubble Interaction (SBI)

As a more practical problem, we chose liquid shock-cylindrical air bubble interaction problem with 175 by 125 mesh. A moving shock of M=1.422 in liquid hits the cylindrical gas bubble of d=2mm. This problem is the modeling of the contribution of gas bubbles near kidney stone in lithotripsy process.

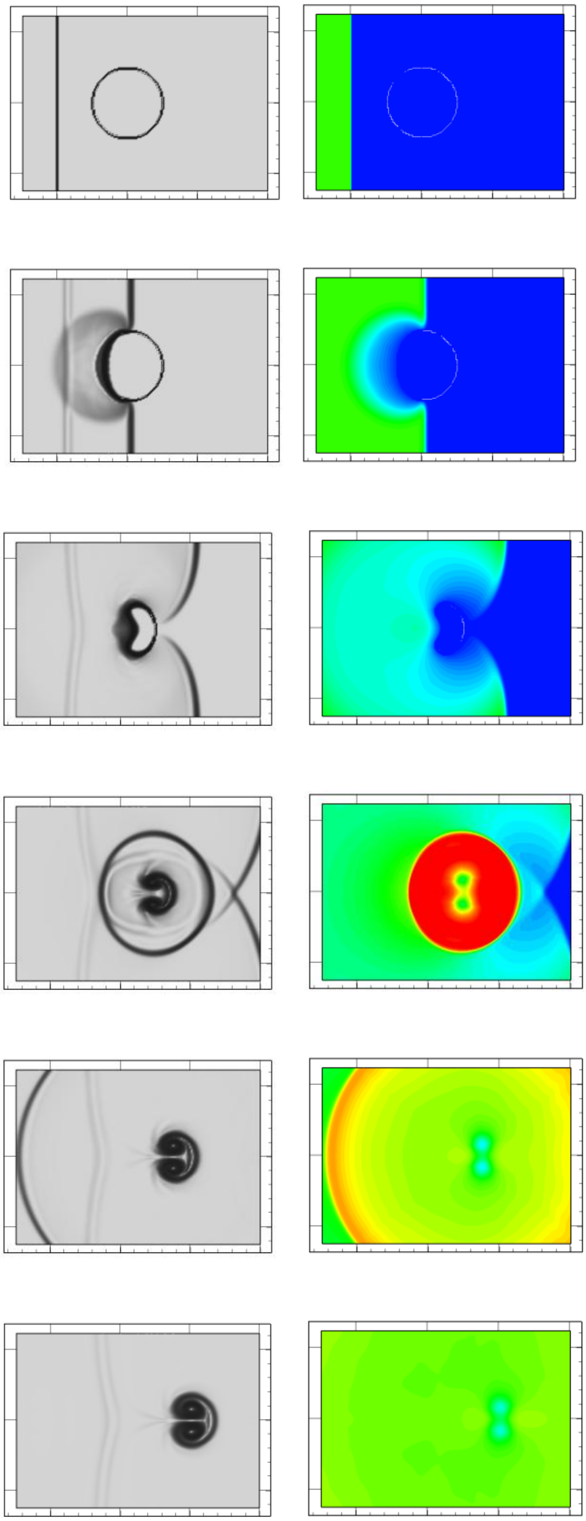

Fig. 5 Shock-bubble interaction at every 0.1μs
(left: numerical schlieren of density, right: pressure)

As we can see in section 6.2, when the liquid shock hits gas bubble, reflection wave is a rarefaction wave, while incident wave is still a shock. However, when the transmitted shock coincides with gas-to-liquid phase interface, both reflection and incident waves are all shock waves. So the blasting wave is generated at the right end of the gas bubble. And we can see the high-speed liquid jet between the vortex pair which is formed after the bubble collapse. Numerical results show well-known flow physics including blast wave and liquid jet formation in Fig. 6.

7. CONCLUSION

Numerical methods for simulating compressible two-phase flows with large density ratio are presented. We extended the RoeM and AUSMPW+ scheme which are recently developed for gas dynamics to two-phase flows. For the two-phase flows using homogeneous equilibrium model (HEM) with mass fraction, shock discontinuity sensing term (SDST) is derived from mixture EOS. New shock discontinuity sensing term has the value of 1/O(1) even for the near liquid phase. The developed two-phase versions of RoeM and AUSMPW+ schemes are tested on several air-water two-phase problems. In spite of the large discrepancy of material properties, the numerical results show a good performance of the developed schemes. We expect that our proposed shock discontinuity sensing term can be used for other numerical applications for two-phase flows. And let us mention that both the SDST and the developed schemes have a consistent form for isothermal compressible two-phase flows.

ACKNOWLEDGMENTS

The authors appreciate the financial support by the Brain Korea-21 Program for the Mechanical and Aerospace Engineering Research at Seoul National University.

REFERENCES

[1] S. S. Kim, C. Kim, O. H. Rho, S. K. Hong, "Cures for the shock instability: Development of a shock-stable Roe scheme," *J. Computational Physics*, Vol. 185, pp. 342-374, 2003.

[2] K. H. Kim, C. Kim, and O. H. Rho, "Methods for the Accurate Computations of Hypersonic Flows, Part I: AUSMPW+ Scheme," *J. Computational Physics*, Vol. 174, pp. 38-80, 2001.

[3] S. Venkateswaran, J. W. Lindau, R. F. Kunz, C. L. Merkle, "Computation of Multiphase Mixture Flows with Compressibility Effects," *J. Computational Physics*, Vol. 180, pp. 54-77, 2002.

[4] Robin K. S. Hankin, "The Euler Equations for Multiphase Compressible Flow in Conservation Form," *J. Computational Physics*, Vol. 172, pp. 808-826, 2001.

[5] H. Luo, J. D. Baum, R. Lohner, "On the computation of multi-material flows using ALE formulation," *J. Computational Physics*, Vol. 194, pp. 304-328, 2004.

[6] K. H. Kim, J. H. Lee, O. H. Rho, "An Improvement of AUSM Schemes by Introducing the Pressure-Based Weight Functions," *Computers and Fluids*, Vol. 27, No. 3, pp. 311-346, 1998.