Upwind Scheme Using Preconditioned Artificial Dissipation for Unsteady Gas-liquid Two-phase Flow and Its Application to Shock Tube Flow

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ABSTRACT

A stable upwind finite-difference method for unsteady gas-liquid two-phase flows is proposed and applied to shock tube flows. The artificial dissipation terms in the flux difference splitting upwinding scheme are derived using a preconditioned matrix to enhance the stability and convergence of the numerical calculation of mixed compressible and incompressible flows with arbitrary void fractions. A homogeneous gas-liquid two-phase flow model is used. A stable four-stage Runge-Kutta method and the flux difference splitting upwind scheme combined with a third-order MUSCL TVD scheme are employed. Using the proposed method, we compute gas-liquid mixture shock tube problems and compare their results with the exact solution to check the reliability of the proposed method. Shock and expansion wave propagations through the gas-liquid two-phase media are observed in detail. The effect of the preconditioned artificial dissipation on the numerical stability and convergence rate are investigated. We confirm that the proposed method is stable and effective for computations of unsteady two-phase complex flows with arbitrary Mach numbers.

1. INTRODUCTION

Gas-liquid two-phase flow is frequently encountered in engineering problems such as cavitation, boiling, aerosol applications, and sloshing of cryogenic fluids. Taking cavitating flow as an example, when a cavitating bubble occurs and collapses near the surface of a body, it causes noise and vibration, damaging the hydraulic machine system. Therefore, for these unfavorable phenomena to be reduced, accurate prediction and estimation of the two-phase flow are very important. Hence, cavitating flow models for numerical simulations (Deshpande et al., 1997; Singhal et al., 1997; Merkle et al., 1998) as well as analytical and experimental methods (Tomita et al., 1986; Bourne et al., 1992) for shock-bubble interaction problems have been proposed to understand the behavior of collapsing cavitation bubbles. However, owing to the strong and complicated unsteady flow phenomena such as phase change, the co-existence of compressible and incompressible flow, vortex shedding, and turbulence in cavitating flow, mathematical expressions of the flow and development of numerical methods have not been established yet. Recently, Shin et al. (2003) proposed a mathematical cavitating flow model based on a homogeneous equilibrium model while considering the compressibility of gas-liquid two-phase media. With this model, detailed mechanisms of the development of cavitation have been investigated using cavitating flow problems (Seo et al., 2008; Dittakavi et al., 2010). These schemes have also been extended to preconditioned dual time-stepping methods to solve both unsteady compressible and incompressible flow associated with a very large range of sound speeds, which can occur in cavitating flows with various rates of void fractions (Shin et al., 2004).

This paper extends previous high-resolution schemes (Shin, 2011) with the third-order MUSCL TVD scheme to a stable time consistent method to solve unsteady gas-liquid two-phase flow with arbitrary Mach numbers. For a stable and accurate treatment of gas-liquid interfaces considered with discontinuity, artificial dissipation terms in the flux splitting on the upwinding are modified using a preconditioning matrix that is usually applied to the time derivative term to solve very-low Mach number flow using a compressible flow solver (Chorin, 1967; Choi & Merkle, 1993). Gas-liquid two-phase shock tube problems with arbitrary void fractions are computed to provide...
Numerical examples. The applicability of the method to the unsteady problem is demonstrated, and unsteady shock wave phenomena, including the propagation of both compression and expansion waves, are investigated.

2. NUMERICAL METHODS

2.1 Fundamental Equations

The fundamental equations used in this paper are the one-dimensional (1-D) Euler equations for the mixture mass, momentum, energy, and gas-phase mass conservation (Shin, 2011), and they are expressed as follows:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \]

with \( Q = \begin{bmatrix} \rho \\ \rho u \\ e \\ \rho Y \end{bmatrix} \) and \( E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e + p)u \\ \rho u Y \end{bmatrix} \) (1)

where, \( \rho, u, e, Y, \) and \( p \) in the unknown variable vectors \( Q \) and flux vectors \( E \) are the mixture density, velocity, total energy, quality of vapor and pressure, respectively. In this paper, Eq.(1) is solved using a finite-difference method based on a compressible flow solver. Additionally, the equation of state derived using thermodynamic relations, \( p = \rho c^2(T + \rho c) \) (Shin et al., 2003) was used for gas-liquid two-phase flow, as shown in Eq. (2).

\[ \rho = \frac{p(\gamma^p + \gamma)}{K(1-\gamma)p(T + \gamma) + RT(p+\rho c)^2} \] (2)

In this equation of state, \( T \) represents temperature, \( R \) is the gas constant, and \( K, p_c, \) and \( T_c \) represent the liquid, pressure and temperature constants for water, respectively. In this two-phase flow model, the apparent compressibility is considered, and the speed of sound \( c \) is exactly derived using thermodynamic relations, \( c^2 = \rho c_p / (\rho + \rho c_p \rho_p) \) (Shin et al., 2004, 2011). Here, \( C_p \) is the specific heat capacity at a constant pressure of the gas-liquid two-phase medium. \( \rho_T \) and \( \rho_p \) represent \( \partial \rho / \partial T \) and \( \partial \rho / \partial \rho \), respectively.

2.2 Preconditioning Matrix

Gas-liquid two-phase flow, such as cavitating flow, has both compressible and incompressible flow characteristics. For such flows, a compressible flow solver that can solve the incompressible flow is advantageous. Hence, artificial compressible methods and preconditioning methods (Chorin, 1967; Kwak et al., 1984; Choi & Merkle, 1993) have been developed and used in steady state computation. Generally, preconditioning methods are not acceptable for time dependent problems because the time derivative is multiplied by the preconditioning matrix known as the preconditioner. Therefore, this preconditioning method for steady problems was later improved to a time-consistent method through a dual time-stepping procedure (Shuen et al., 1992; Venkateswaran & Merkle, 1995; Shin et al., 2004) and used for unsteady flow calculations. However, although this dual time-stepping preconditioning method is useful in solving unsteady flow while maintaining temporal accuracy, it requires long computing times to obtain an unsteady solution.

In this paper, a stable and effective upwind numerical scheme that reduces computing time for unsteady gas-liquid two-phase flow is proposed by applying preconditioning. In other words, instead of dual time-stepping, by modifying only the artificial dissipation term in an upwind scheme using a preconditioning matrix without changing the time derivative term, we propose an unsteady solution method that is always consistent in time.

The preconditioning matrix can be derived through various methods (Turkel, 1986; Choi & Merkle, 1993; Weiss & Smith, 1994), but it is usually derived using primitive variables because the system of equations and the computation of the Jacobian matrix of the system are simplified. To obtain the preconditioning matrix with the primitive variable, the conserved variable \( Q \) in Eq.(1) is transformed into primitive variable \( W \) using the following transformation matrix \( \Gamma_w^{-1} \):

\[ \Gamma_w^{-1} \frac{\partial W}{\partial t} + \frac{\partial E}{\partial x} = 0 \]

with \( W = [p, u, T, Y]^T \) and \( \Gamma_w^{-1} = \frac{\partial Q}{\partial W} \) (3)

In order to solve both compressible and incompressible flow problems using compressible flow schemes, the transform matrix \( \Gamma_p^{-1} \) in Eq.(3) must be modified by a preconditioning matrix. Therefore, in this study, as introduced in a previous work (Shin et al., 2004), the preconditioning matrix \( \Gamma_p^{-1} \) is derived by adding the vector \( \theta [1, u, H, Y]^T \) to the first column of matrix \( \Gamma_w^{-1} \) (Weiss & Smith, 1994; Edwards & Liou, 1997) concretely as

\[ \Gamma_p^{-1} = \begin{bmatrix} \theta + \rho_p & 0 & \rho_T & \rho_Y \\ u(\theta + \rho_p) & \rho & u_{\rho_T} & u_{\rho_Y} \\ H(\theta + \rho_p) - 1 & \rho u & \rho c_p + H \rho_T & H \rho_Y \\ Y(\theta + \rho_p) & 0 & Y \rho_T & \rho + Y \rho_Y \end{bmatrix} \] (4)
where $H$ is enthalpy defined by total energy $e = \rho H - p$. 
The preconditioning parameter $\theta$ is defined as $\frac{1}{\alpha^2} - \frac{1}{c^2}$
with a switching parameter $a^2 = \min[c^2, \max(|u|, \beta |U|)]$, $\beta$ is a constant, $U_0$ is a fixed reference velocity
designed to prevent a singularity at the stagnation point in compressible and incompressible flows (Weiss & Smith, 1994; Edwards & Liou, 1997).

### 2.3 Preconditioned Numerical Flux

In contrast, to achieve a stable computation of high-speed and complicated multiphase flow, we must also stabilize the solution method, including the upwinding of the advection terms. In the present method, Roe’s approximate Riemann solver is applied to increase the stability. According to Roe’s flux-difference splitting (FDS) scheme (Roe, 1981), the derivative of the flux vector $E$ in Eq.(3) can be expressed as $(\partial E/\partial x)_{i} = (E_{i+1/2} - E_{i-1/2})/\Delta x$, and the numerical flux $E_{i+1/2}$ is approximated as

$$E_{i+1/2} = \frac{1}{2}(E(Q_{i+1/2}^{L}) + E(Q_{i+1/2}^{R})) - |A|_{i+1/2}(Q_{i+1/2}^{R} - Q_{i+1/2}^{L}) \quad \text{(5)}$$

In Eq.(5), the Roe matrix $|A|_{i+1/2}$ is an artificial dissipation or artificial viscosity consisting of the flux Jacobian matrix $A(= \partial E/\partial Q)$ for numerical stability in upwinding processes, and it is evaluated by the Roe-average. Because Eq.(5) is originally designed for compressible flow, it is unsuitable for computing very-low Mach number flow owing to the stiff problem (Choi & Merkle, 1993; Turkel et al., 1994; Koren & van Leer, 1995). Therefore, in this paper, to overcome this problem and solve complex flows with a large range of Mach number such as gas-liquid two-phase flows, we modify the flux Jacobian matrix $A$ to a preconditioned flux Jacobian matrix $\tilde{A}$ that applies the preconditioning matrix $\Gamma_p^{-1}$ obtained above. This modification requires that Eq.(3) is preconditioned first and then rewritten in preconditioned hyperbolic form in terms of primitive quantities $W$ via linearization of the flux vector as follows:

$$\Gamma_p^{-1} \frac{\partial W}{\partial t} + \frac{\partial E}{\partial x} = 0 \quad \text{(6)}$$

Moreover, in the hyperbolic system of $W$ after the linearization of $\partial E/\partial x$ with Jacobian matrix, we obtain

$$\frac{\partial W}{\partial t} + A_p \frac{\partial W}{\partial x} = 0 \quad \text{(7)}$$

where, $A_p = \Gamma_p \bar{A} \Gamma_p^{-1}$, and $\Gamma_p$ is the inverse matrix of $\Gamma_p^{-1}$.

In the upwinding, the advection term of the system $W$ is transformed back into a conservative system of variables $Q$ to improve the conservation properties and the ability to capture the shock interface of the gas-liquid medium. Therefore, the derivative of the flux vector $\partial E/\partial x$ for applying Roe’s FDS can be transformed by using $A_p$ as

$$\frac{\partial E}{\partial x} = \Gamma_p^{-1} A_p \Gamma_p \frac{\partial Q}{\partial x} = \bar{A} \frac{\partial Q}{\partial x} \quad \text{(8)}$$

where, $\Gamma_p$ is the inverse matrix of $\Gamma_p^{-1}$.

In Eqs.(7) and (8), because the preconditioned matrix $A_p$ has real eigenvalues, it can be diagonalized in the form $A_p = L_p \Lambda_p L_p^{-1}$. Eventually, the preconditioned numerical flux $E_{i+1/2}$ corresponding to Eq.(5) is approximated as follows:

$$E_{i+1/2} = \frac{1}{2}(E(Q_{i+1/2}^{L}) + E(Q_{i+1/2}^{R})) - |A_p|_{i+1/2}(Q_{i+1/2}^{R} - Q_{i+1/2}^{L}) \quad \text{(9)}$$

where, $\Lambda_p$ in the artificial dissipation term is a diagonal matrix of the preconditioned characteristic speeds (eigenvalues), and $L_p$ is the matrix consisting of the left eigenvectors of $A_p$, derived as follows:

$$\Lambda_p = 
\begin{pmatrix}
\text{diag}(\frac{\partial Q}{\partial x})
\end{pmatrix}
$$

In the preconditioning matrices of Eq.(9), at $\theta = 0$ without preconditioning, the apparent speed of sound $\pm c$ becomes $\pm c$, and the eigenvalues and eigenvectors of the preconditioned flux Jacobian matrix are returned to their traditional form of $A$ for compressible flow in Eq.(5). As mentioned in the previous section, because $\theta$ is controlled according to the type of flow and the stiff problem is also eliminated, Eq.(6) employing the preconditioned numerical flux of Eq.(8) can solve flows with both compressible and incompressible flow characteristics (Weiss & Smith, 1994; Edwards & Liou, 1997). Additionally, because the stability term can be appropriately constructed considering the accuracy and stability of numerical schemes, $\Gamma_p^{-1}$ in the third term of Eq.(9) could be replaced by $\Gamma_w^{-1}$.

### 2.4 Riemann Variables $Q^{LR}$

Riemann variables $Q^{LR}_{i+1/2}$ in Eq.(9) are constructed using primitive variables $W^{LR}_{i+1/2}$, which are obtained by applying the MUSCL TVD scheme (van Leer, 1979) as follows:

$$W^{LR}_{i+1/2} = W_i + (1/4)(1 - \kappa) D^+ W_{i-1/2} + (1 + \kappa) D^- W_{i+1/2}$$

$$W^{L}_{i+1/2} = W_i - (1/4)(1 - \kappa) D^- W_{i+1/2} + (1 + \kappa) D^+ W_{i+1/2} \quad \text{(10)}$$

Here, the flux-limited values of $D^\pm W$ and the minmod function are determined as

$$D^+ W_{i-1/2} = \minmod(\delta W_{i-1/2}, b \delta W_{i+1/2})$$

$$D^- W_{i+1/2} = \minmod(\delta W_{i+1/2}, b \delta W_{i-1/2})$$

$$\delta W_{i+1/2} = W_{i+1} - W_i$$
In Eq.(10), the linear combination parameter $\kappa$ and the limiter $b$ that controls the slope of the flux in the minmod function are selected according to the accuracy of the scheme and the TVD stability condition (Shin, 2003). In the third-order MUSCL TVD scheme of this paper, $\kappa$ of 1/3 and $b$ of 4 are applied.

### Time Integration

As mentioned in Sec.2.2, because preconditioning the time-derivative term destroys the time-consistency, the fundamental equations that preserve the original time-derivative terms must be time integrated to obtain the time-consistent solution in the unsteady flow problem. Therefore, in this paper, instead of the conventional preconditioned equation (6) suitable for steady-state low-speed flow computations, we propose the fundamental equations (3) with the primitive unknown variable, in which only the artificial dissipation term is preconditioned by applying equation (8) while maintaining time consistency. Thus, this numerical method always provides a time-consistent solution, unlike the conventional preconditioning methods (Turkel et al., 1994; Liou & Edward, 1999; Shin et al., 2004).

In implementing the time integration of Eq.(3), we use the following four-stage explicit Runge-Kutta method (Jameson & Baker, 1983) in a finite difference discretization. This method has fourth-order accuracy for a linear equation and does not require storing intermediate solutions.

\[
\begin{align*}
W^1 &= W^n - \Delta t/4L_\nu L(Q^n) \\
W^2 &= W^n - \Delta t/3L_\nu L(Q^n) \\
W^3 &= W^n - \Delta t/2L_\nu L(Q^n) \\
W^{n+1} &= W^n - \Delta t_\nu L(Q^n)
\end{align*}
\]

(11)

Here, the superscript $n$ denotes $n$-th time level, $L(Q)$ (= $\partial E/\partial x$) is the preconditioned flux term of Eq.(8) and $L_\nu$ ($= \partial W/\partial Q$) is the transform matrix. The time integration of Eq.(11) yields a time accurate solution for unsteady problems, and can more properly simulate the behavior of pressure and propagation of acoustic waves in incompressible flow (Weiss & Smith, 1994) and multiphase flows because the primitive variables are directly obtained as unknown variables. The stability and efficiency of the present numerical method described thus far are confirmed through numerical experiments for unsteady gas-liquid two-phase shock tube problems in the following section.

### 3. NUMERICAL RESULTS

The present numerical method has been validated using 1-D Riemann problems (Laney, 1998) with different initial conditions. The computational domain of $x$ is [-10 m, 10 m]. The initial conditions of the left ($L$-) and right ($R$-) hand sides separated by a discontinuity at $x = 0$ m for two test cases are given in Table 1. In all test cases, the temperature, velocity, and void fraction are set to $T = 300$ K, $u = 0$ m/s and $\alpha = \alpha_i$, and density $\rho$ is initially imposed using Eq.(2). Case 1 is a standard Sod’s test problem (Sod, 1978), and Case 2 is a test problem with a very large pressure ratio to check numerical stability and convergence rate, which are typical shock tube problems.

Figure 1 shows the computational results of the pressure, velocity, density, and temperature distributions of Case 1 for an ideal gas ($\alpha_i = 100\%$) with the ratio of specific heats $\gamma = 1.4$ at times (a) $t = 5$ ms, (b) 10 ms, (c) 15 ms, and its exact solutions (Laney, 1998). The time evolution results obtained using the present method of the third-order MUSCL TVD scheme using preconditioned numerical fluxes of Eq.(9) and 100 grids adequately simulate the propagation of the shock and expansion waves over time from the initial position to the right and left, respectively. Additionally, the results obtained using 10,000 grids (black solid line) completely overlap with the exact solutions (red solid line). The results for another gas phase flow in Case 2 at $t = 10$ ms are shown in Fig.2. Although Case 2 is a very difficult test problem containing a very large pressure ratio of 100 in the initial conditions, the present method performs a stable computation without a large initial jump at the discontinuity. The results obtained using 10,000 grids completely overlap with the exact solutions, and the results using 100 grids are simulated fairly well, except for the presence of relatively small dissipation at the discontinuity.

Based on the validity of the present method confirmed thus far, the present method is applied to the two-phase shock tube problems with an arbitrary void fraction $\alpha_i$, and the characteristics of pressure waves propagating in the gas-liquid mixed medium are investigated. As an example of two-phase flow, Figs.3 to 7 (a) show computational results of pressure, velocity, density, and void fraction distributions, and (b) show their iteration histories of maximum residuals of $|p^{n+1} - p^n|_{\text{max}}$ and $|u^{n+1} - u^n|_{\text{max}}$ for Case 2 at different initial void fractions. Here, to investigate the applicability of the present method, including accuracy and stability under a very severe computational condition, we select Case 2 involving an exceedingly large pressure ratio and analyze it using a complex multiphase flow in which the speed of sound changes with the change in the void fraction. In figure (a), the black solid lines indicate the results obtained via Roe’s first-order upwind scheme using a very fine grid of 100,000 to account for numerical stability and reduce the smearing and dissipation of the contact; these are considered an exact solution for the two-phase shock tube flow because no reference data are available. The red solid lines and symbols represent the results obtained using the
(a) at time $t = 5$ ms

(b) at time $t = 10$ ms
Fig. 1 Time evolution results of pressure, velocity, density, and temperature for unsteady numerical solutions at 5, 10, and 15 ms for gas phase flow at $\alpha_i = 100\%$ (Case 1)

(c) at time $t = 15$ ms

Fig. 2 Computational results of pressure, velocity, density, and temperature distributions for gas phase flow at $\alpha_i = 100\%, t = 10$ ms (Case 2)
third-order MUSCL TVD scheme using the numerical flux of Eq. (5) and the preconditioned numerical flux of Eq. (9) with 100 grids, respectively.

Moreover, in figure (b), the black and red solid lines show the iteration histories in the computation with and without the preconditioned numerical flux, respectively. As these figures show, the present method using preconditioned numerical flux predicts unsteady two-phase shock tube problems fairly well for all test cases with the void fraction between 80% and 20%. Overall, the result without preconditioned numerical flux exhibits strong overshoots and oscillations near discontinuities in pressure and velocity distributions, whereas the preconditioned numerical flux does not. The iteration histories of the maximum residuals of pressure and velocity also show that introducing preconditioning to the numerical stability term improves both the convergence rate and stability compared with no preconditioning. The effect of preconditioning on numerical stability is greater.
at lower void fractions of the flow, that is, at a higher liquid content. Thus, the present method with preconditioned numerical flux is more stable and provides more accurate results than those without preconditioning.

On the other hand, as for the flow phenomenon of gas-liquid two-phase shock tube flow, as the shock wave propagates, the void fraction decreases to almost a liquid state because the shock wave compresses the two-phase medium, but the expansion wave shows the opposite behavior. The contact discontinuities occur and move to the right-hand side with the wave-induced velocity. These phenomena can be inferred from changes in density. The wave induced velocity decreases rapidly in two-phase media and decreases as the initial void fraction decreases. It can also be seen that the pressure behind the shock wave decreases rapidly.
is higher than that of the single-phase gas flow shown in Fig. 2. Such flow phenomena are characteristics of shock tube problems in gas-liquid mixed media.

Similar to the two-phase flow described above, computational results for a single-phase liquid flow with the void fraction $\alpha_i = 0\%$ at $t = 3.4$ ms are shown in Fig. 8. The legend and grids in the computation are the same as those in Figs. 3-7. In this case, because single-phase flow is considered, the present method with preconditioning performs relatively numerically stable computations and predicts pressure, velocity, density, and temperature distributions of the liquid phase flow very well. For this flow, the present high-resolution method without preconditioning obtains almost the same results as with preconditioning. Even in the same single-phase flow, expansion waves are propagating like compression waves in the liquid phase unlike the gas phase flow in Fig. 2. This

Fig. 5 Comparisons of pressure, velocity, density, and void fraction distributions, and iteration histories for gas-liquid mixture flow at $\alpha_i = 50\%, t = 0.375$ s (Case 2)
is due to the large difference between the speed of sound in the liquid and the velocity induced by the waves (Shin, 2011). Moreover, variations in velocity, density, and temperature are very small compared with that of the single-phase gas flow.

4. CONCLUSIONS

A stable upwind finite-difference method for unsteady gas-liquid two-phase flow is proposed and applied to the two-phase shock tube problem. In this
method, the artificial dissipation term in the flux difference splitting is derived using the preconditioning matrix to improve the numerical stability. In order to obtain a time-consistent solution, we integrate the fundamental equations using primitive variables as the unknown variable with preconditioning imposed only on the flux term using a stable four-stage Runge-Kutta method combined with a third-order MUSCL TVD scheme. A homogeneous equilibrium model of gas-liquid two-phase flows is used.

We confirmed that time-consistent results such as pressure, density, velocity, and temperature distributions obtained using the present method for ideal gas agree with the exact solutions. Additionally, the present method simulates the gas-liquid mixture shock tube flow well.
without losing time consistency. Moreover, we observe that the preconditioned flux term significantly increases both the numerical stability and convergence rate in unsteady flow computations compared with those without preconditioning. The improvement in stability is more pronounced for two-phase flows with both compressible and incompressible flow characteristics than for single-phase flow. The reliability and applicability of the present method to unsteady flow problems with arbitrary void fraction and speed of sound are demonstrated. To further investigate the validity and applicability of the proposed method, we plan to extend it to multidimensional gas-liquid actual flow problems.

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The authors declare that they have no competing interests.

AUTHORS CONTRIBUTION
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REFERENCES


