Unified CFD approach to simulate two-phase flows in presence of surface forces

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Abstract— In this paper the diffuse interface model for direct numerical simulation of liquid-vapor interfaces in the presence of surface in presented. This model is developed from two-phase compressible flow approaches known as relaxation-projection method for compressible flows, simple and efficient relaxation method using pressure non-equilibrium model. The model accounts for the phase compressibility and surface tension effects and adapted for simulation of the bubble and drop flows. Results of testing of numerical technique are presented and demonstrate the good perspective of developed approach for simulation of multi-phase flows.

Keywords— CFD, relaxation-projection method, surface force, two-phase flows.

I. INTRODUCTION

The liquid–vapor flows with phase change are often encountered in industrial applications such as nuclear reactors, heat exchangers, boilers, etc. Their better understanding requires experimental investigations as well as the development of analytical models. To develop analytical models and to help interpret experimental data and understand local physical phenomena the direct numerical simulations can be used. The use of the direct numerical simulation is already quite common in single-phase fluid dynamics. The numerical problems encountered to simulate two-phase flows with phase change are much more complicated. The tracking of a surface of discontinuity on a fixed numerical grid is a base complexity in these numerical problems. Several methods proved their efficiency to solve this problem; the most common ones are the volume-of-fluid [1], front-tracking [2], and level-set methods [3]. These methods mainly deal with immiscible fluid systems. In such systems, the speed of displacement of an interface is equal to the velocity of the fluids (gas and liquid) at the interface. Therefore, knowing the velocity field, it is quite easy to interpolate it at the interface and move the interface accordingly. When phase change exists, the problem is more complicated because three different velocities exist at an interface: the velocities of the liquid and vapor phases and the speed of displacement of the interface.

Liquid–vapor phase change effects have been resolved within the one-fluid formulation by different researchers: Beux with colleagues [4] used the LS method; Jamet [5] applied the so-called second gradient theory or the Cahn–Hilliard equations.

During of the last ten years numerical methods and algorithms for solving of the heat and mass transfer problems in compressible/incompressible fluids were developed. Among these are algorithms for solving of incompressible fluid dynamics, algorithms for solving of compressible fluid dynamics at the low Mach numbers, the monotone multidimensional schemes for solving of an advection equation, an effective algorithm for solving of elliptical equation for pressure correction. These methods and algorithms were applied successfully for computational support of the experiments financed by Nuclear Energy Agency at Organization of Economic Cooperation and Development within the MASCA project [6], where a behavior of the two non-mixing liquids, such as corium and steel was investigated. Now these computing tools will be extended on a case of two-phase flows as a gas-liquid system.

For incompressible/compressible two-phase flows unified CFD approach was developed [7] which is based on the developed algorithms with small scheme diffusion, where the discrete approximations are constructed with use of finite-volume methods and fully staggered grids. For modeling of 3D turbulent single-phase flows LES approach (commutative filters) was used. For modeling of 3D turbulent two-phase flows by means DNS the enough detailed grids and effective numerical methods developed in IBRAE for solving of CFD problems were applied. For observation of an interface of two-phase flow the modified VOF methods and multidimensional transfer schemas of TVD-type with small scheme diffusion with use of sub-grid simulation were used.

A considerable number of modern simulation methods of multiphase and multicomponents gas dynamics flows are based on the numerical solution of Euler or the Navier-Stokes equations which are usually supplemented by one or several equations expressing conservation laws of specific physical values to given problem (concentration of gas bubbles), it is
necessary for definition of interface parameters for multiphase system.

Application of such numerical methods leads to occurrence of artificial diffusivity through contact discontinuity and to artificial mixing of substances on interface. In such artificial mix of value of all thermodynamic parameters are calculated with an error. With strongly differing parameters of substances such approach leads to negative values of pressure already on the second step on time. The two-phase model has been offered in Abgral and Sauvel’s paper [8], which allowing defining thermodynamic and kinetic variables of each component of a mix. Thus in any place of a calculated grid the identical equations were solved by means of the same numerical method as for a case of two not mixing components separated by an interface, and for a case of presence of physical mixing of various substances.

The diffuse interface model for direct numerical simulation of liquid-vapor interfaces in the presence of surface forces was developed from two-phase compressible flow approaches known as relaxation-projection method for compressible flows, simple and efficient relaxation method using pressure non-equilibrium model. The model accounts both the phase compressibility and surface tension effects and adapted for simulation of the bubble and drop flows. Results of testing of numerical technique speak about the good perspective of developed approach for simulation of multi-phase flows.

The possibility of using diffuse interface model for direct numerical simulation of liquid-vapor interfaces in the presence of surface forces is used to test numerical technique. This model was developed by using Hamilton’s principle of stationary action [9]. Numerical technique is based on adapted HLLC Riemann solver [10] supplemented with simple and efficient relaxation method using pressure non-equilibrium model [11]. Such approach was used for simulation of the bubble and drop flows.

Generalization for phase transition modeling can be achieved by natural physical processes splitting with relaxation and phase transition [12].

\[
\frac{\partial \rho_1}{\partial t} + \nabla \cdot (\rho_1 \mathbf{u} ) = 0; \\
\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \mathbf{u} ) = 0; \\
\frac{\partial \rho_1}{\partial t} + \nabla \cdot (\rho \mathbf{u} ) = 0; \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u} ) = 0; \\
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} ) = - \frac{1}{\rho} \nabla \cdot \mathbf{P}; \\
\frac{\partial \mathbf{P}}{\partial t} + \nabla \cdot (\mathbf{P} \mathbf{u} ) = 0; \quad \Phi = \frac{1}{2} \mathbf{e} \cdot \mathbf{e}; \\
\frac{\partial \mathbf{e}}{\partial t} + \nabla \cdot (\mathbf{e} \mathbf{u} ) = \frac{1}{\rho} \nabla \cdot \mathbf{P}.
\]

The hyperbolicity of the model (3) is shown in [12]. To solve it numerically several disadvantages have to be taken into account [11].

Main among these disadvantages concerns with non monotone behavior of the equilibrium sound speed with respect to the volume fraction. Also non-conservative volume fraction equation could yield to positivity preserving difficulties when rarefaction or compression waves are present at interfaces.

To avoid such disadvantages pressure non-equilibrium model is used. With this approach system (3) will take form:
where \( p_I \) – interface pressure.

At first step the hyperbolic part of the system (4) is solved:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + u \cdot \nabla \rho &= 0, \\
\frac{\partial u}{\partial t} + u \cdot \nabla u &= 0, \\
\frac{\partial (\rho u)}{\partial t} + \nabla (\rho u u) &= 0, \\
\frac{\partial (\rho e)}{\partial t} + \nabla (\rho e u) &= 0,
\end{align*}
\]

\[
\begin{align*}
\frac{\partial (\rho u)}{\partial t} + \nabla (\rho u u) &= 0, \\
\frac{\partial (\rho e)}{\partial t} + \nabla (\rho e u) &= 0, \\
\frac{\partial (\rho u)_{1} \rho}{\partial t} + \nabla (\rho u_{1} \rho u) &= -p_I \rho \mu \times (p_I - p_2), \\
\frac{\partial (\rho u_{2} \rho)}{\partial t} + \nabla (\rho u_{2} \rho u) &= -p_I \rho \mu \times (p_I - p_2).
\end{align*}
\]

Next relaxation step forces the solution of pressure non-equilibrium model (5) to converge to that of the equilibrium model (3). This step is fulfilled for the system:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + u \cdot \nabla \rho &= \mu (p_1 - p_2), \\
\frac{\partial u}{\partial t} + u \cdot \nabla u &= 0, \\
\frac{\partial (\rho u)}{\partial t} + \nabla (\rho u u) &= 0, \\
\frac{\partial (\rho e)}{\partial t} + \nabla (\rho e u) &= 0, \\
\frac{\partial (\rho u)_{1} \rho}{\partial t} + \nabla (\rho u_{1} \rho u) &= -p_I \rho \mu \times (p_I - p_2), \\
\frac{\partial (\rho u_{2} \rho)}{\partial t} + \nabla (\rho u_{2} \rho u) &= -p_I \rho \mu \times (p_I - p_2)
\end{align*}
\]

where \( p_I \) – interface pressure.

III. NUMERICAL TECHNIQUE

The main point is that the numerical algorithm does not look for the liquid-vapor interfaces, and it is identical in the whole calculated region.

In the absence of relaxation terms the conservative part of system (5) are updated with conversational Godunov scheme:

\[
U_{i,j}^{n+1} = U_{i,j}^{n} - \frac{\Delta t}{\Delta x} \left( F_{i+1/2,j}^{n} (U_{i+1,j}^{n} - U_{i,j}^{n}) - F_{i-1/2,j}^{n} (U_{i,j}^{n} - U_{i-1,j}^{n}) \right)
\]

where upper script * stands for the perturbated state,

\[
U = (\rho, \rho u, \rho v, \rho E, \rho X, \rho Y, \rho \Phi, \rho \Psi, \rho Z)
\]

\[
F_{x} = (\rho u, \rho u^2, w, u_w, p, \rho u_{2}, \rho u_{2}, psi_{2}, \alpha_{2} p_{1}, \alpha_{2} p_{2}) - \lambda w \times \left( 1 - \frac{w^2}{w^2} \right) \rho u_{2} + \frac{w^2 w_{y}^{2}}{w} \rho u_{2}^2 + \alpha_{1} p_{1} + \alpha_{2} p_{2} - \lambda w \times \left( 1 - \frac{w^2}{w^2} \right)
\]

The volume fraction is calculated using the Godunov method for advection equation that guarantees volume fraction positivity during the hyperbolic step:

\[
(\alpha_{1})_{i,j}^{n+1} = (\alpha_{1})_{i,j}^{n} - \frac{\Delta t}{\Delta x} \left( (u_{1} \alpha_{1})_{i,j+1}^{n} - (u_{1} \alpha_{1})_{i,j-1}^{n} \right) - \frac{\Delta t}{\Delta y} \left( (u_{1} \alpha_{1})_{i,j}^{n+1} - (u_{1} \alpha_{1})_{i,j}^{n-1} \right)
\]

The non-conservative energy equations are updated with simplest approximation by assuming the product \((\alpha_{1} p_{1})_{i,j}^{n}\) constant during time step:

\[
(\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j}^{n+1} = (\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j}^{n} - \frac{\Delta t}{\Delta x} \left( (\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j+1}^{n} - (\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j-1}^{n} \right) - \frac{\Delta t}{\Delta y} \left( (\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j}^{n+1} - (\alpha_{1} p_{1} \alpha_{1} e_{1})_{i,j}^{n-1} \right)
\]

The lack of accuracy in the internal energy computation will be corrected on the relaxation step in agreement with the second law of thermodynamics.

To determine the values of thermodynamic variables for perturbated state the adaptation of HLLC solver was performed. The left- and right- facing waves speeds along X and Y directions are obtained as following:

\[
\begin{align*}
(S_{L})_{x} &= \max \left( u_{L} + (c_{L})_{x} \right) - \min \left( u_{L} + (c_{L})_{x} \right), \\
(S_{L})_{y} &= \max \left( u_{L} + (c_{L})_{y} \right) - \min \left( u_{L} + (c_{L})_{y} \right), \\
(S_{R})_{x} &= \max \left( u_{R} + (c_{R})_{x} \right) - \min \left( u_{R} + (c_{R})_{x} \right), \\
(S_{R})_{y} &= \max \left( u_{R} + (c_{R})_{y} \right) - \min \left( u_{R} + (c_{R})_{y} \right),
\end{align*}
\]

where \( c^2 = \frac{y^2 c_1^2 + y^2 c_2^2}{y^2} \) – frozen sound speed.
The speeds of intermediate waves or contact discontinuities are estimated as:

\[ u_x^* = (S_M)_x = \left\{ \rho u_x^2 + p - \lambda w \left( 1 - \frac{w_x^2}{w^2} \right) \right\}_L - \left\{ \rho u_x^2 + p - \lambda w \left( 1 - \frac{w_x^2}{w^2} \right) \right\}_R - (S_L)_x \rho_L (u_x)_L + (S_R)_x \rho_R (u_x)_R \} / (\rho u_x L - (\rho u_x)_L - (S_L)_x \rho_L + (S_R)_x \rho_R) \]

\[ u_y^* = (S_M)_y = \left\{ \rho u_y^2 + p - \lambda w \left( 1 - \frac{w_y^2}{w^2} \right) \right\}_L - \left\{ \rho u_y^2 + p - \lambda w \left( 1 - \frac{w_y^2}{w^2} \right) \right\}_R - (S_L)_y \rho_L (u_y)_L + (S_R)_y \rho_R (u_y)_R \} / (\rho u_y L - (\rho u_y)_L - (S_L)_y \rho_L + (S_R)_y \rho_R) \]

From above wave speeds the variable states are determined:

\[ (\rho^*_R)_x = (\rho_R)_x \times \frac{(S_R)_x - (u_x)_L}{(S_R)_x - (S_M)_x}, \]

\[ (\rho^*_R)_y = (\rho_R)_y \times \frac{(S_R)_y - (u_y)_L}{(S_R)_y - (S_M)_y}, \]

\[ (\rho^*_L)_x = (\rho_L)_x \times \frac{(S_L)_x - (u_x)_R}{(S_L)_x - (S_M)_x}, \]

\[ (\rho^*_L)_y = (\rho_L)_y \times \frac{(S_L)_y - (u_y)_R}{(S_L)_y - (S_M)_y}, \]

\[ (w^*_R)_x = (w_R)_x \times \frac{\rho^*_R}{\rho_R}, \]

\[ (w^*_L)_x = (w_L)_x \times \frac{\rho^*_L}{\rho_L}, \]

\[ (w^*_R)_y = (w_R)_y \times \frac{\rho^*_R}{\rho_R}, \]

\[ (w^*_L)_y = (w_L)_y \times \frac{\rho^*_L}{\rho_L}, \]

\[ p^*_i = (p_R)_i + (\rho_R)_i \times ((u_i)_R)_i \times \left( \left( (u_i)_R \right)_i - (S_R)_i \right) + (S_M)_i \left( S_R - (S_M)_i \right) + (S_M)_i \left( S_R - (S_M)_i \right) + \lambda \times \left( \frac{w_R^2}{w_R^2} \right)_i \]

\[ + \lambda \times \left( \frac{w_R^2}{w_R^2} \right)_i - \lambda \times \left( w_R^2 \right)_i \times \left( \frac{w_R^2}{w_R^2} \right)_i \]

\[ p^*_y = (p_R)_y + (\rho_R)_y \times (u_y)_R \times \left( \left( (u_y)_R \right)_y - (S_R)_y \right) + (S_M)_y \left( S_R - (S_M)_y \right) + \lambda \times \left( \frac{w_R^2}{w_R^2} \right)_y - \lambda \times \left( w_R^2 \right)_y \times \left( \frac{w_R^2}{w_R^2} \right)_y \]

The volume fraction jump is constant along fluid trajectories in the absence of relaxation effects:

\[ (\alpha^*_x)_R = (\alpha_x)_R, \]
\[ (\alpha^*_y)_R = (\alpha_y)_R, \]

\[ (\alpha^*_x)_L = (\alpha_x)_L, \]
\[ (\alpha^*_y)_L = (\alpha_y)_L. \]

The internal energy jump conditions for stiffened EOS \( p_k = (\gamma_k - 1) \rho_k e_k - \gamma_k \pi_k \), \( k = 1, 2 \) provide the following relations:

\[ p_k^* = (p_k + \pi_k) \times \left( (\gamma_k - 1) \rho_k - (\gamma_k + 1) \rho_k^* - \pi_k \right), \]

\[ k = 1, 2. \]

\[ \pi_k^* = p_k \times \gamma_k \]

Approximate Riemann solvers (7)-(15) allow to apply described Godunov scheme. Extension to second order can be done with MUSCL type method. In this approach the predictor step is fulfilled for primitive variables with a half time interval. New values for primitive variables are used then in HLLC solver to update system (5) in corrector step.

Relaxation step for pressure non-equilibrium model can be reduced from system (6) to a couple of equations:

\[ e_k \left( \frac{p_k - p_k^0}{\rho_k^0} - e_k^0 \right) + \rho_k \times \left( \frac{1}{\rho_k^0} - \frac{1}{\rho_k} \right) \times p_k = 0, \]

\[ k = 1, 2. \]

where \( p_I \) - interface pressure, which can be evaluated as \( p_I = p \) or \( p_I = p^0 \); superscript 0 means initial state before relaxation.

To find unknown variables: \( p, \rho_1, \rho_2 \) one closure relation is needed. For this purpose saturation constraint is used:

\[ \alpha_1 + \alpha_2 = \frac{(\alpha_0 \rho_1^0 + \alpha_0 \rho_2^0)}{\rho_1 + \rho_2} = F(p) = 1 \]

IV. COMPUTATIONAL RESULTS

In all computations the liquid is governed by the stiffened gas equation of state with parameters: \( \gamma_{liq} = 2.1, \pi_{liq} = 10^7 \) Pa. The gas is governed by the ideal gas equation of state with polytropic exponent \( \gamma_{gas} = 1.4 \).
A. Round droplet

A round water droplet with radius \( R = 0.11 \text{m} \) placed in air. The pressure is \( 10^5 \text{ Pa} \) everywhere outside the droplet. Inside the droplet the pressure is \( 10^5 + \frac{\lambda}{R} = 10^5 + \frac{1000}{0.11} = 109090 \text{ Pa} \) according to Laplace law. The mesh with 100 \times 100 cells was used. The pressure profiles for initial instant and after 100000 calculation steps are shown in Fig. 1. The scheme retains the pressure jump with error which is lower than 10\% comparing with the value from Laplace law.

![Fig. 1. The pressure profiles for initial instant and after 100000 calculation steps.](image)

B. Oscillating square droplet

A square water droplet placed in air. The pressure is \( 10^5 \text{ Pa} \) everywhere in the computational domain. The mesh with 100 \times 100 cells was used. The initial position of the square droplet is shown in Fig. 2 using gas volume fraction profile.

The droplet becomes to decrease its surface energy due to surface tension effects which are characterized by the parameter \( \lambda = 1000N/m \). This induces the oscillations up to equilibrium state.

Results of calculations are presented in Fig. 3 at different instants \( t_1 = 26 ms, \ t_2 = 53 ms, \ t_3 = 79 ms, \ t_4 = 106 ms \). At steady state the droplet has a circular shape of radius 0.13 m with an average surplus pressure 7010 Pa. The error in the pressure jump is lower than 10\% comparing with the value from Laplace law, which is \( \approx 7690 \text{ Pa} \).

![Fig. 2. Initial position of the square droplet.](image)

![Fig. 3. Oscillation of the square droplet due to surface tension effects at different instants.](image)

C. Oscillating Ellipsoid Bubble

An ellipsoid gas bubble with axis ratio 1:1.5 placed in water. The pressure is \( 10^5 \text{ Pa} \) everywhere in the computational domain. The mesh with 100 \times 100 cells was used.

The initial position of the ellipsoid bubble is shown in Fig. 4 using gas volume fraction profile.

The bubble becomes to decrease its surface energy due to surface tension effects which are characterized by the parameter \( \lambda = 1000N/m \). This induces the oscillations up to equilibrium state.

Results of calculations are presented in Fig. 5 at different instants \( t_1 = 43 ms, \ t_2 = 68 ms, \ t_3 = 145 ms, \ t_4 = 183 ms \). At steady state the bubble has a circular shape of radius 0.135 m

![Fig. 4. Initial position of the ellipsoid bubble.](image)

![Fig. 5. Oscillation of the ellipsoid bubble due to surface tension effects at different instants.](image)
with an average surplus pressure 6750 Pa. The error in the pressure jump is lower than 10% comparing with the value from Laplace law, which is $\approx 7400$ Pa.

**Fig. 4.** Initial position of the ellipsoid bubble.

**Fig. 5.** Oscillation of the ellipsoid gas bubble due to surface tension effects at different instants.

**D. Gas Bubble Surfacing In Liquid**

A round gas bubble initially is placed at the bottom part of solid vertical tube, filled by the water.

The pressure profile is stratificated from $10^5$ Pa at lowest section of the tube according to the gravity force action (see Fig. 6).

**Fig. 6.** Initial position of the gas bubble in solid tube (up) with stratificated profile of the pressure (down).

Gas bubble begins to surface due to the density gradient in gravity field and changes the form due to surface tension effects which are characterized by the parameter $\lambda = 2 N/m$.

Bubble positions at different instants ($t_1 = 0.28 s, t_2 = 0.82 s, t_3 = 1.37 s, t_4 = 2.06 s$) are shown in Fig. 7 using gas volume fraction profile.
E. Propagation of pure capillary standing wave

A water and vapor sinusoid interface is located at the middle part of the square domain with solid walls.

The pressure is $10^5$ Pa everywhere in the computational domain. The mesh with $150 \times 150$ cells was used.

The initial position of the interface is shown in Fig. 8 using water mass and volume fraction profiles.

The surface tension and dynamic viscosity coefficients are $\lambda = 1000 \, N/m$ and $\nu = 6 \, Pa \times s$.

The simulation results provided for pure capillary waves with viscosity effects are presented in Fig. 9 at different instants ($t_1 = 0.16 \, s$, $t_2 = 0.29 \, s$, $t_3 = 0.46 \, s$, $t_4 = 0.59 \, s$) using water mass fraction profile.

V. CONCLUSION

Results of testing of numerical technique speak about the good perspective of developed approach for multi-phase flow simulation.
REFERENCES


