MODEL FOR THE SIMULATION OF THE INTERFACE DISPERSION

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ABSTRACT

Two models - basically different in their treatment of the two-phase flow - are coupled together to simulate transients with the dispersion of the interface. The Volume of Fluid (VOF) model, uses an interface-tracking algorithm for the simulation of the two-phase flow, can be used only as long as a local grid density allows surface tracking. Second model -"two-fluid" model - is based on less accurate equations averaged in time and space and does not track the interface explicitly and is more suitable for simulations of dispersed flow. A Rayleigh-Taylor instability is used as a representative problem for the test of the coupled model, where long time development of the instability causes mixing of the fluids and dispersion of the interface. Grid refinement studies are made to examine the mechanism of the switch between models and to check the convergence of the physical characteristic.

1 INTRODUCTION

Two-phase flow plays an important role in many natural and industrial processes such as combustion, petroleum refining, chemical engineering, nuclear technology and others [7]. The numerical simulations are important tool for the investigation of the two-phase flow. They has given a significant contribution to the understanding of the two-phase flow characteristics and vice versa – the variance and complexity of the two-phase flow stimulate the development of many different mathematical models and numerical tools for its simulation.

The interface tracking methods, which are used for simulations of transients with moving discontinuous interfaces [2] are the basic two-phase flow models from the standpoint of the Navier-Stokes equations. Since they are based on the fundamental Navier-Stokes equations they explicitly track the interface. During the calculation they keep the interface
sharp and enable the accurate location of the particular fluid at any time during the transient. Such an approach allows direct simulations of the two-phase flow phenomena like the phase change and surface tension [4]. The interface tracking algorithms were applied to numerous phenomena, which simulations showed also one obvious limitation of the interface tracking models: none of the simulations mentioned above crossed the point, where the discrete grid could not follow the dispersion of the interface. In a dispersed flow, where chunks of the particular fluid are smaller than the grid cells, the surface tracking is not possible and the method fails.

Since most of two-phase flows of practical importance are too dispersed to be resolved with the interface tracking algorithms, it is clear that different approaches are necessary. So-called "two-fluid" models, based on different techniques of time, spatial or statistical averaging [3], which resulted in similar "two-fluid" model equations. Despite the weakness common to all averaging schemes - a lack of knowledge of the closure relations - two-phase flow modeling will not be possible without the averaged models in the foreseen future.

This work presents the coupling of both models, which retains the accuracy of the interface tracking schemes for a simple two-phase flow and eliminates the need for the special closure relations of the two-fluid models for the same simple flow. When the flow is dispersed and the interface tracking becomes impossible, a relatively accurate "two-fluid" model is available. Among many different well-established interface algorithms the VOF method is assumed to be the most convenient, because the color function in the VOF model and volume fraction in the "two-fluid" model actually represent the same variable. This variable represents the basis of the proposed coupling mechanism.

2 MODELS INVOLVED IN COUPLING

2.1 Model Based on VOF Method

A model based on the VOF method is suitable for describing two-phase problems, where the characteristic length of the interface shape is larger than the grid size. This model describes the two-phase flow by the Navier-Stokes system consisting of a continuity and momentum balance equation. For the two-dimensional system of incompressible viscid fluids the following continuity and momentum equations are usually used [6]:

\[ \nabla \cdot \mathbf{\dot{u}} = 0, \quad \rho \frac{\partial \mathbf{\dot{u}}}{\partial t} + \rho (\mathbf{\dot{u}} \cdot \nabla) \mathbf{\dot{u}} = \rho \mathbf{g} - \nabla p + \nabla \cdot (\mu \mathbf{D}), \]

where \( \mathbf{\dot{u}}=(u(x,y,t), v(x,y,t)) \) is a 2D velocity field, \( p=p(x,y,t) \) is a pressure field, \( D=(\nabla \mathbf{\dot{u}} + \nabla \mathbf{\dot{u}}^T)/2 \) is a viscous stress tensor and \( \mathbf{g} \) is a gravity. Both fluids are treated with the same equations, where the density \( \rho(x,y,t) \) and the viscosity \( \mu(x,y,t) \) are functions of space and time denoting either the first or the second fluid.

The interface tracking in the VOF method is based on the color function \( f(x,y,t) \) [6], which has the value \( I \) on the place of the first fluid and \( \theta \) on the place of the second one. On the discrete grid the mesh cells, which contain both fluids, this function has the value of the volume fraction one of the fluid, which is \( 0< f_{\text{mixed}}<1 \). Among several reconstruction algorithms the LVIRA algorithm [6] is used for the reconstruction of the interface in our work. This algorithm makes a linear approximation of the interface by putting a line segment in each multi-fluid cell, i.e., in each cell which has \( 0< f_{i,j} < 1 \). The approximate interface
orientation in the cell \((i,j)\) is determined from the volume fractions in a 3x3 block of neighboring cells. The orientation of each interface segment is determined by the normal vector \(\vec{n}\), which is calculated by the minimization of the function

\[
G_{i,j}(\vec{n}) = \sum_{l=-1}^{1} \sum_{k=-1}^{1} (f_{i+k,j+l} - f'_{i+k,j+l}(\vec{n}))^2 .
\]  

An example of this algorithm is shown in Figure 1 where the fluid 1 is signed with the dark color and the fluid 2 with the white one. The values of \(f_{i+k,j+l}\) are known volume fractions of the fluid 1 in a 3x3 block of cells. The values of \(f'_{i+k,j+l}(\vec{n})\) are the volume fractions (hatched area) due to the line with the normal \(\vec{n}\) (dotted line in Figure 1), which divides the block on two parts and conserves the volume fraction in the center cell of the block, i.e., \(f_{i,j} = f'_{i,j}\).

### 2.2 "Two-Fluid" Model

The "two-fluid" models are suitable for two-phase problems, where the length scale of the interface shape is smaller than the grid size. The basic assumption of those models is that each fluid as a continuum occupies the whole domain. Information lost by the averaging are replaced by more or less accurate closure relationships for the interfacial transfer of mass, momentum and energy provided empirically mostly from experiments. This approach is more suitable for simulations of the dispersed flow. The continuity and momentum equations for the system of incompressible viscous fluids used in the present model are [5]

\[
\frac{\partial f_k}{\partial t} + \nabla \cdot (f_k \vec{u}_k) = 0 , \quad f_k \rho_k \frac{\partial \vec{u}_k}{\partial t} + f_k \rho_k \vec{u}_k \nabla \vec{u}_k = f_k \rho_k \vec{g} - f_k \nabla p + C_k (\vec{u}_k - \vec{u}_l) + f_k \nabla (\rho_k \vec{D}_k) .
\]  

The two fluid system is described with two systems of Eqs. (3) with \(k=1\) for the fluid 1 and \(k=2\) for the fluid 2. Both fluids are regarded as two mixed phases that share space in proportion to their volume fraction, which satisfy the equation \(f_1 + f_2 = 1\) and the same pressure. At any location there is a pair of velocities, which interact with the exchange of momentum. One kind of interfacial transfer of momentum is interfacial friction, which is described empirically coefficient \(C_k\). In our case the correlation for the laminar flow is used [5]: \(C_1 = -C_2 = c_d \bar{\rho} f_1 f_2\), where \(c_d\) is an empirical constant and \(\bar{\rho} = \rho_1 + \rho_2\) is the mixture density. Since the volume fraction in the “two-fluid” model has a similar meaning as the color function (3) in the VOF model, the same symbol "f" is used.

![Figure 1: Interface reconstruction with the LVIRA algorithm](image)

![Figure 2: Coupling of two-fluid and VOF area](image)
3 COUPLED MODEL

The continuity and momentum equations of both models (1), (3) are discretized and solved on a rectangular two-dimensional domain covered. The time integration and the finite difference approximation of the equations is similar as in the MAC method [1].

The coupled model is designed to simulate on the same calculation domain the area where the fluids are mixed and calculated with the “two-fluid” model (lighter gray area in Figure 2) and the area where the fluids are separated and calculated with the VOF model (black and white areas in Figure 2). Each mesh cell is assigned to one model - to the VOF model or "two-fluid" model. The cells, which contain only one fluid, are automatically in the VOF domain. The essential problem of the coupling is a choice of a switch criterion, which would choose the model that will be used in mixed cells- cells that contain both fluids. Since the kind of model applied to the particular place depends on the local dispersion of the fluids, the criterion must estimate the local dispersion of the interface around the particular cell. In our work the dispersion function in the cell \((i,j)\) is defined as:

\[
\gamma_{i,j} = \min(G_{i,j}(\vec{n})).
\]  

The function \(G\) defined by Eq. (2), which was originally developed for the calculation of the interface segment orientation in the LVIRA interface reconstruction algorithm, turns out to be useful also for the estimation of the local dispersion. A dispersion function \(\gamma\) checks the positions of the fluids in the \(3\times3\) block of cells with the respect to the best-estimated linear interface. The perfect non-dispersed state is achieved when the fluids are separated with the linear interface, when the dispersion function is zero, i. e., \(\gamma=0\). If a part of the fluid is located on the "wrong" side of the linear interface, then \(\gamma>0\). The dispersion function is used for the declaration of the switch parameter \(\gamma_0\), which states:

\[
\begin{align*}
\text{if } \gamma_{i,j} < \gamma_0, & \text{ the interface in the cell } (i,j) \text{ is reconstructed with VOF model} \\
\text{if } \gamma_{i,j} > \gamma_0, & \text{ the fluids in the cell } (i,j) \text{ are calculated with the "two-fluid" model}
\end{align*}
\]  

In order for proper determination of the parameter \(\gamma_0\) and efficient coupling of the model, the main characteristics of \(\gamma\) have to be analyzed. Firstly, dispersion \(\gamma\) can be split into two parts:

- I: Reconstruction of a single interface that cuts the \(3\times3\) block of cells into two parts results in a nonzero dispersion \(\gamma\), when the original interface is not linear.
- II: The second type of dispersion appears when two chunks (bubbles) of the dispersed fluid approach to a distance close to the grid size (Figure 5 and Figure 6).

I. One of the most common topological shapes in two-phase flow is a bubble, which is used for the examination of the part I of dispersion \(\gamma\). Figure 3 shows a circular bubble with a center in the point \(S(x,y)\) and with \(d/h\) diameter to the grid spacing ratio. The cells, which are cut by the interface of the circle have each a little different value of dispersion. An ideal parameter for measuring the dispersion should have a constant value for all positions of the bubble. However, it is probably impossible to construct such a parameter. All relative positions of the bubble were checked by moving the center of the circle \(S\) within a single mesh cell (Figure 3- hatched area) to find the cell with the maximal dispersion \(\gamma_{max}\). The Figure 4 shows the dependence of maximal dispersion from the bubble diameter to grid size ratio \(d/h\). Larger \(d/h\) ratio means more grid cells per bubble and results in smaller values of the dispersion \(\gamma\). The Figure 4 shows rapid increase of \(\gamma\) values for diameters \(d\) less then approximately \(2h\) to \(3h\). This result is in agreement with the fact, that at least three grid cells per bubble diameter are needed to capture its circular shape with some minimal accuracy, and justifies the choice of \(\gamma\) as a measure of the interface dispersion.
The result in Figure 4 allows to set a threshold value $\gamma_0$: setting $\gamma_0 = \gamma_{\text{max}}$ determines the minimal characteristic size of the bubble, which can be simulated with the VOF method. For example: setting $\gamma_0 = 0.6$ means that the bubble or a part of the surface with the characteristic size $d > 4h$ are treated with the VOF model. Smaller chunks with dispersion $\gamma_{\text{max}} > \gamma_0$ and might be still treated with the VOF model, since dispersion depends on the surface to mesh relative position. But as they move over the discrete grid, the dispersion in some cell on the interface sooner or later exceeds the parameter value $\gamma_0$ and switches the cell to the "two-fluid" model.

II. The second kind of dispersion, when two chunks of fluid approach to each other to a distance comparable to the grid spacing, is shown in Figure 5 and Figure 6. The hatched area shows the volume, which contributes to $\gamma$. In some cases the LVIRA algorithm may still correctly reconstruct the interface (Figure 5). But if the interfaces are too close, the reconstruction may fail - the Figure 6 shows the case when the interface (thick line) in the middle cell is positioned on the wrong side of the cell. The detailed analyses of the reconstruction failure [8] showed that any reconstruction error provides dispersion which is larger than $\gamma > 0.4$. If the switch parameter is set to $\gamma_0 = 0.4$ then no reconstruction error occurs in the VOF model, because such cells are switched to the "two-fluid" model.

According to the presented results $\gamma_0 = 0.4$ was used as a value of the threshold parameter $\gamma_0$. This value ensures that the chunks with the characteristic size $d > 5h$ are treated with the VOF model and no reconstruction error occurs in the simulation.

4 RESULTS

Comparison of results obtained with the coupled model and real experimental data is possible only partially: like the numerical methods, which are designed for the simulations of the dispersed or stratified flow, the experiments are also specialized for the examination of a
particular flow type. Among several basic two-phase flow phenomena, the Rayleigh-Taylor instability turns out to be the most suitable for the assessment of the coupled model, since during the transient the two-phase flow changes from stratified to dispersed and vice versa.

In the initial state of the phenomenon, the heavier fluid $\rho_1=3$ lies above the lighter one $\rho_2=1$ in a channel with the width $l$ and height $5$. The sinusoidal disturbance of the interface with the amplitude $0.002$ is increased due to gravity acceleration $g=10$. Both fluids have the same kinematic viscosity $\nu_1=\nu_2=10^{-2}$. Figure 7 shows the VOF simulation performed with different grid densities. The heavier fluid is marked with black color and the lighter one is white. The VOF method successfully describes the initial states of the instability (Figure 7a) especially on the finest grid. Further development of the phenomenon disperses the fluids (Figure 7b). For such dispersed state even the finest grid does not give the realistic description of the phenomenon - the VOF results are different for each grid density.

![Figure 7: Rayleigh-Taylor instability at time a) $t=1.6$ and b) $t=8$ with VOF method](image)

The grid dependence is investigated with the comparison of the volume fraction fields simulated on two different grids:

$$\delta_{nod}(t)=\frac{1}{N} \sum_{(i,j)\in V} \left( f_{gridA}(t) - f_{gridB}(t) \right)^2,$$

where $f_{gridA}$ is a volume fraction field calculated on a coarser grid, $f_{gridB}$ is a volume fraction calculated on a finer grid and interpolated on the coarser grid A in the calculation domain. Figure 8 shows the temporal development of the $\delta_{nod}$ function for several pairs of grids. In the initial phase of the transient higher resolution gives more accurate results (lower $\delta_{nod}$) since there is no dispersion. However, after certain time interval, when the fluids are well mixed, all VOF simulations end with non-acceptable reconstruction errors and no convergence on the denser grid is observed.

![Figure 8: Temporal development of the $\delta_{nod}$ function](image)

Figure 10 shows the time development of the instability simulated with the coupled model. In the initial stages the VOF model calculates the transient. Once the "two-fluid" model is activated, it is spread all over the calculation domain due to the vortexes, which appear during the transient. In the final stages of the transient, mixing of the fluids is replaced by the stratification process, which leads to the reverse process - construction of the new interface and activation of the VOF model between the lighter and the heavier fluid.
Since the correct solution of the problem is not known and there is a lack of experiments, which would give appropriate data, the evaluation appeared to be a rather difficult task. The simplest procedure for the evaluation of the coupled model is comparing of the volume fraction distributions with the Eq. (6). The distribution of the volume fraction in the second part of the transient ($t>5$) depends mainly on the interfacial friction constant $c_d$ (3). On the other hand the volume fraction distribution in the pure VOF model appeared to depend also on the grid density. With the variation of the interfacial friction constant $c_d$ in the coupled model it is possible to match the result of pure VOF model on every grid density. Therefore the volume fraction distribution from the simulation with the pure VOF method with the $48x240$ mesh density was used as an orientation (bulk) solution. Although this bulk solution is not accurate, it is used for comparison with the coupled model. The value of the interfacial friction constant $c_d=40$ is chosen to match the simulations of the coupled model to the simulation with the VOF bulk solution on the grid $48x240$ as close as possible.

The purpose of such comparison is to prove that the coupled model is useful on all grid densities - also on the coarse grid. The volume fractions of the coupled model and "bulk" solution are interpolated on a $6x30$ grid to smooth the discrete structures of the VOF model and are compared on the basis of the $\delta_{nod}$ variable (Eq.(6)). The Figure 9 shows the time history of $\delta_{nod}$ for several grid densities. Calculations with the coupled model using different grid density give a relatively small variation of the volume fraction distribution compared to the pure VOF simulation, which is also added to the Figure 9. The coarsest $6x30$ grid gives worse agreement compared to the pure VOF model at the beginning ($t<2$). That is because the coupled model calculates that part of the transient mostly with "two-fluid" model, while it can be accurately calculated with the VOF model on a higher resolution ($24x120$ for example). Beside that the value of the interfacial friction coefficient $c_d=40$ is probably not correct for that part of the transient. Denser grids give better agreement because coupled model uses the VOF model longer. Later ($t>5$), when the fluids disperse, all the grid densities give better
approximation, because the fluid motion in the pure VOF model depends on the reconstruction algorithm, which is not valid at that state.

5 CONCLUSIONS

The coupling of a simple VOF model and a "two-fluid" model was used for the simulation of the two-phase problem with the dispersion of the interface. The coupled model exploits particular characteristics of both models: accurate simulation of the interface with the VOF model and relatively small grid dependence of the "two-fluid" model in the dispersed flow. The switch parameter between the models is provided from the function, which is already used by the LVIRA interface reconstruction algorithm in the VOF method. Some simple numerical calculations have shown that the switch parameter $\gamma_0$ around 0.4 is the most proper value to change from the VOF to the "two-fluid" model and vice versa. The switch between the models is based only on the position of the volume fractions, what is a good approximation for the simulated case. For more complex transients it can be upgraded with the physical characteristics and empirical correlations.

The coupled model gives results, which are grid dependent, i. e., denser nodalization does not result in a grid independent solution, but it gives a better approximation. The simulation of coupled model with the coarse grid gives qualitatively the same result as on the finer grid but with a larger error. The simulation of the whole transient of the Rayleigh-Taylor instability, until the fluids exchange their positions, has showed that the coupled model enables more realistic calculation of a wider range of two-phase phenomena than the pure VOF model. However, the problem is a comparison of the coupled model with the experiment, since there are not many experiments investigating the interface-tracking and the dispersion phenomena at the same time.

6 REFERENCES