

A LARGE SCALE INTERFACE MULTIFLUID MODEL FOR SIMULATING MULTIPHASE FLOWS

Vinesh H. GADA^{1*}, Jebin ELIAS¹, Mohit P. TANDON¹ and Simon LO²

¹ CD-adapco, Pune, Maharashtra, India

² CD-adapco, Didcot, Oxfordshire, United Kingdom

*Corresponding author, E-mail address : vinesh.gada@cd-adapco.com

ABSTRACT

The scope of the Eulerian Multiphase (EMP) model in STAR-CCM+ is extended to simulate multi-scale two-phase flows using Large Scale Interface (LSI) model. The LSI model provides a criteria based on local phase-distribution to distinguish between regimes characterized by small and large scale interfaces. An appropriate closure for conserved variable is specified for each regime, weighted sum of which forms the closure for the interaction between the phases. The LSI model also allows to model surface tension effects in the vicinity of large scale interfaces as well. The large scale interface is treated as a moving wall using a turbulence damping procedure near the interface. This extended multifluid methodology implemented in STAR-CCM+ is validated using several standard two-phase flow problems.

NOMENCLATURE

a_s interfacial area density
 g acceleration due to gravity
 k turbulent kinetic energy
 l interaction length scale / particle diameter
 p pressure
 t relaxation time scale
 \vec{u} velocity
 C_D drag coefficient
 \vec{F} interaction force
 I phase pair interactions
 V volume
 W weight function
 \vec{F}_S surface tension force

α volume fraction
 β $k - \omega$ model closure coefficient
 Δ cell quantity
 κ interface curvature
 μ dynamic viscosity
 ω specific dissipation rate
 ρ density
 σ coefficient of surface tension
 τ shear stress

Subscripts

c, d continuous, dispersed phase
 p, s primary, secondary phase
 fr, ir, sr first, interface, second regime
 k k^{th} phase
 r relative
 t turbulent
 D, S drag, surface-tension

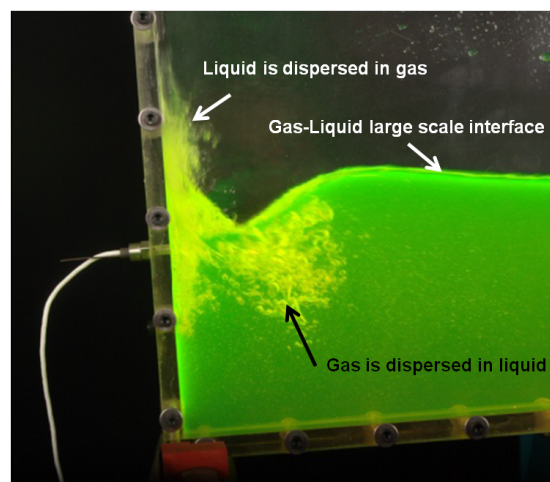


Figure 1: Coexistence of small and large scale interface during sloshing of liquid in a cavity (Souto-Iglesias et al., 2011).

INTRODUCTION

Multiphase flows are found in variety of industrial applications. Such flows are markedly different from single-phase flows due to presence of interface, across which there is jump in fluid-properties as well as mass, momentum and energy interactions occur. For modeling considerations, such flows can be classified based on the increasing spatial scales of interface between the phases, into dispersed (bubbly flow, droplet flow), mixed/intermittent (slug flow, churn flow) and separated/stratified (film flow, annular flow, horizontal stratified flow). In several practical situations, it is likely that these multiphase flow regimes coexist. Sloshing of liquid in partially filled container shown in Figure 1 is one such example of coexistence of multiple multiphase flow regimes. It is seen that, near the cavity wall, some liquid is dispersed in air as well as air is dispersed in liquid; away from the wall a clear large-scale interface is seen.

The volume-tracking/interface-capturing methods such as Volume-Of-Fluid (VOF) or Level-Set (LS) method are well suited for simulation of stratified multiphase flows, where typical interfaces are larger than the grid size. Such interfaces are characterized as large scale interfaces. Since the volume-tracking/interface-capturing methods rely on resolving the interface completely, they are prohibitively expensive for simulating multi-scale flows where modeling dispersed regime physics is critical. The Eulerian Multiphase (EMP) model, also known as the multifluid model, on the other hand, has had good success in these aspects and has been widely used for

simulation of dispersed multiphase flows. The EMP model treats each phase as inter-penetrating continua and each phase is characterized by its own physical properties and velocity field; pressure is shared by the phases. This generality of modeling opens up an opportunity to develop a framework for simulating even separated two-phase flows using EMP model, with appropriate closures being used for Large Scale Interface (LSI) flows.

In the present work, a methodology is developed within the multifluid modeling framework for simulation of dispersed as well as separated two-phase flow. Development of such a method throws several challenges. Firstly, a criterion to classify the two-phase flow into dispersed or separated/large scale interface regime is needed. Thereafter, appropriate closure for momentum and energy should be used for each regime and near the transition boundaries, these closures should be smoothly blended for numerical stability. For dispersed two-phase flow, the effect of surface-tension is included in the interface drag (Tomiya et al., 2002). However, in case of LSI regime, the surface-tension needs to be modeled explicitly. The existence of LSI in separated regime also needs special modeling of turbulence quantities in its vicinity. For a general case of gas-liquid flow, the gas phase sees the interface as a moving wall. Thus, the turbulence needs to be dampened in the vicinity of the large scale interface to capture this effect. In this paper, a systematic approach to each of these challenges is presented in form of the LSI model, implemented in STAR-CCM+. The model is validated on variety of separated two-phase problems: dam-break simulation, Young-Laplace law test, turbulent air-water stratified flow and laminar oil-water stratified flow with heat transfer.

MATHEMATICAL MODEL DESCRIPTION

Eulerian Multiphase (EMP) model treats the contributing phases as interpenetrating continua coexisting in the flow domain. Equations for conservation of mass, momentum, energy and turbulence are solved for each phase (Tandon et al., 2013 and CD-adapco, 2015). The share of the flow domain occupied by each phase is given by its volume fraction and each phase has its own velocity, temperature fields and physical properties. Interactions between phases due to differences in velocity and temperature are taken into account via the inter-phase transfer terms in the transport equations; which provide the closure to the set of equations. In the solution method described here, all the phases share a common pressure field.

GOVERNING EQUATIONS Considering adiabatic flows, the main equations solved here are the conservation of mass and momentum for each phase.

CONTINUITY

The conservation of mass for the k^{th} phase is :

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k) = 0 \quad (1)$$

where α_k , ρ_k and \vec{u}_k is volume fraction, density and velocity of phase k , respectively. The sum of the volume fractions is equal to unity.

MOMENTUM

The conservation of momentum for the k^{th} phase is :

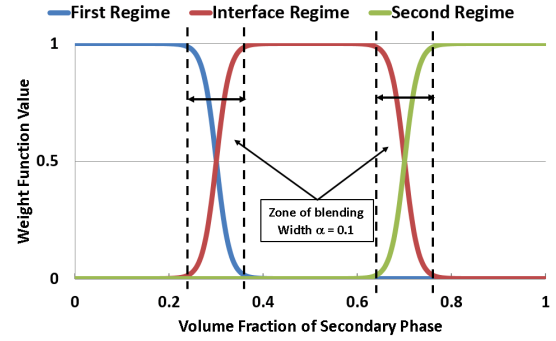


Figure 2: Variation of blending weight functions with volume-fraction of secondary phase in the LSI model

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_k \rho_k \vec{u}_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k \vec{u}_k) - \nabla \cdot (\alpha_k (\tau_k + \tau_{t,k})) \\ = -\alpha_k \nabla p + \alpha_k \rho_k g + \vec{M} \end{aligned} \quad (2)$$

where τ_k and $\tau_{t,k}$ are laminar and turbulent shear stress, respectively. p is pressure, shared by all phases. \vec{M} is the sum of the interfacial forces. In the present work, only drag force is of consequence and its treatment is discussed in detail here. The large scale interface model however allows modeling of other interaction forces such as lift and turbulent dispersion force in an analogous way (CD-adapco, 2015). For a pair of continuous (c) and dispersed (d) phases, the drag force is defined in terms of linearized drag (A_D) and relative velocity between the two phases ($\vec{u}_r = \vec{u}_c - \vec{u}_d$) as:

$$\vec{M} = \vec{F}_D = A_D \vec{u}_r \quad (3)$$

Where, the linearized drag is calculated as $A_D = \frac{1}{8} C_D a_s \rho_d |\vec{u}_r|$. Here, C_D is the drag coefficient, calculated using applicable correlation, $a_s = 6\alpha_d/l_{cd}$ is the total interfacial area per unit volume or interaction area density considering spherical particles and l_{cd} is interaction length scale / particle diameter. In the LSI model, for a pair of phases, three flow topology regimes are defined and for a cell, the linearized drag is composed from the linearized drag of individual regimes; explained in Large Scale Interface Topology Detection section.

LARGE SCALE INTERFACE TOPOLOGY DETECTION

In the Large Scale Interface Model, it is desired to simulate both dispersed as well as separated two-phase flow. The first step in this direction is the ability to classify the flow into dispersed or separated. This is a complex question and no direct technique is available to do this.

Previously researchers have used volume-fraction based criteria (Tenter et al., 2005; Egorov et al., 2004) to detect flow topology. In the present work, one such simple flow topology detection method is adopted. In this technique, three flow topology regimes are defined for a pair of primary (p) and secondary (s) phases, based on volume-fraction of secondary phase: For $0 < \alpha_s < \alpha_{fr}$ - *First Regime*, where secondary phase is dispersed in primary phase. For $\alpha_{fr} \leq \alpha_s \leq \alpha_{sr}$ - *Large Scale Interface (LSI) Regime*, where both the phases are separated and for $\alpha_{sr} < \alpha_s < 1$ - *Second Regime*, where primary phase is dispersed in secondary phase. To understand this topology definition more clearly, consider a system of water and air as primary phase and secondary phase, respectively. In this scenario, the LSI model will treat

bubbly flow in the first regime, droplet flow in the second regime and separated water-air flow in the LSI regime.

The two thresholds, first regime terminus (α_{fr}) and second regime onset (α_{sr}) gives the flexibility to control the extent sub-topology. α_{fr} is the value of α_s , across which the first regime transits to LSI regime and α_{sr} is the value of α_s , across which the LSI regime transits to second regime. For the present work, their value is taken as $\alpha_{fr} = 0.3$ and $\alpha_{sr} = 0.7$.

These classification of regimes are enforced in every computational cell by calculating the composite interaction using weighted average of linearized drag for each regime.

$$I = \sum_{r=fr,ir,sr} [W_r I_r] \quad (4)$$

where, I are phase-pair interactions such as linearized drag (A_D). The weight functions for each regime calculated as $W_{fr} = 1/(1+\exp(C(\alpha_s-\alpha_{fr})))$, $W_{sr} = 1/(1+\exp(C(\alpha_{sr}-\alpha_s)))$ and $W_{ir} = 1 - (W_{fr} + W_{sr})$. These functions are plotted in Figure 2; Note that, away from the transition thresholds, the weight-functions reduce to 0 or 1. Whereas close to transition boundaries, they vary smoothly between 0 and 1. Also, the width of the transition between two regimes is close to $\alpha = 0.1$. For the first as well as second regime the calculation of phase-pair interactions i.e. linearized drag or heat-transfer are analogous to a general case of continuous-dispersed phase interaction, except for the fact that in first regime, primary-phase is considered as the continuous phase and vice-versa in second regime, secondary-phase is considered as the continuous phase. These sub-topology regimes therefore need, two interaction length scales, l_{ps} and l_{sp} for first and second regime, respectively. For the *water-air* phases, l_{ps} and l_{sp} refer to typical bubble and droplet diameter, respectively. The calculation of linearized drag for LSI regime is discussed in following section.

LARGE SCALE INTERFACE DRAG

In the vicinity of large scale interface, the assumption of spherical interface shape no longer is valid. Several (Frank, 2005; Coste, 2013 and Höhne & Mehlhoop, 2014) approaches have been proposed to model the drag in LSI regime. Physically, for the LSI regime, where the scale of the interface is nearly of the order of cell size, the large scale interface drag should lead to reduced inter-phase velocity-slip. In the present work, method of Štrubelj and Tiselj (2011) is adapted to calculate interface linearized drag coefficient. This form of the interface linearized drag coefficient ensures that the phase occupying larger volume in the cell imparts force to the other phase. The large scale interface linearized drag coefficient is expressed as:

$$A_{D,ir} = \frac{1}{t_{ir}} \alpha_p \alpha_s \rho_m \quad (5)$$

where t_{ir} is the relaxation time-scale. In the present work, a low value (0.01 s) of t_{ir} is used to ensure instantaneous equalizing of velocities of both the phases. Note that, the value of t_{ir} can be modified to change the velocity slip in the vicinity of large scale interface based on the problem at hand.

LSI SURFACE TENSION MODEL

The surface tension force is an interfacial force, which is modeled as volumetric force using the Continuum Surface Force (CSF) approach Brackbill et al., (1992). For a single-velocity formulation (e.g. VOF method), the

surface tension force, more specifically interfacial tension force is calculated as:

$$\vec{F}_S = \sigma \kappa \delta \hat{n} = \sigma \kappa \nabla \alpha_p \quad (6)$$

where, σ is the coefficient of surface/interfacial tension, $\kappa = -\nabla \cdot \hat{n}$ is the interface curvature, $\delta = |\nabla \alpha_p|$ is the interfacial area density and $\hat{n} = \nabla \alpha_p / |\nabla \alpha_p|$ is the unit interface normal; the subscript p denotes the primary phase of the phase-interaction. Štrubelj et al., (2009) proposed the extension of CSF model for multifluid model by splitting the surface-tension force among the phases occupying the cell as $\vec{F}_{S,k} = \phi_k \vec{F}_S$, where subscript k indicates k^{th} phase and ϕ_k denotes the splitting factor of the surface tension force. The pressure gradient within the multifluid model is calculated by summation of momentum equations: $\sum_k \alpha_k \nabla p = \nabla p = \sum_k \phi_k \vec{F}_S$. At kinetic equilibrium, the pressure gradient should be equal to surface tension force, thus: $\sum_k \phi_k = 1$. Štrubelj et al., (2009) showed that use of $\phi_k = \alpha_k$ is better than other alternatives, thus the surface-tension source term in present work is implemented as:

$$\vec{F}_{S,k} = \alpha_k \sigma \kappa \nabla \alpha_p \quad (7)$$

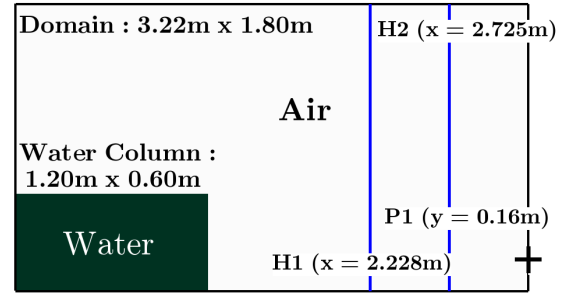


Figure 3: Initial conditions and different probe locations for dam-break simulation.

LARGE SCALE INTERFACE TURBULENCE DAMPING

In the vicinity of large scale interface, a boundary layer develops and flow is close to laminar. Egorov (2004) suggested use of low Re wall like treatment to model turbulence near the large scale interface. This is achieved by enforcing the specific dissipation rate (ω) near the large scale interface as:

$$\omega_{i,k} = T \frac{6\mu_k}{\beta \rho_k \Delta n^2} \quad (8)$$

where subscript k is for k^{th} phase and Δn is the normal distance from interface; which is difficult to calculate in general. Here, Δn is estimated from the cell volume as $\Delta n = \sqrt[3]{\Delta V}$. Note that, the use of Δn instead of exact distance makes this approach different as compared to wall treatment used for actual computational boundaries, this treatment is referred as wall-like treatment. To enforce a Dirichlet condition $\omega_k = \omega_{i,k}$ near the large scale interface, a source term $S_{\omega,k} = a_{ir} \Delta n \beta \rho_k (\omega_{i,k})^2$ is added to specific dissipation rate equation of the phases, where $a_{ir} = 0.5 |\nabla \alpha_p| |\nabla \alpha_s| / (|\nabla \alpha_p| + |\nabla \alpha_s|)$ is large scale interface interaction area density, ensuring that the source term is only added in the vicinity of large scale interface. Since, turbulent viscosity scales as k/ω , high value of ω near

the large scale interface leads to reduction of μ_t and effectively leads to laminarization of flow. The magnitude of ω in the large scale interface region is controlled by the turbulent damping constant T whose recommended value is taken to be at least 100 as demonstrated by Lo & Tomasello (2010) for VOF method.

VALIDATION CASES

The LSI model is validated on three standard test cases; each case is selected to highlight different capability of the approach : drag formulation, turbulence damping model and surface-tension model.

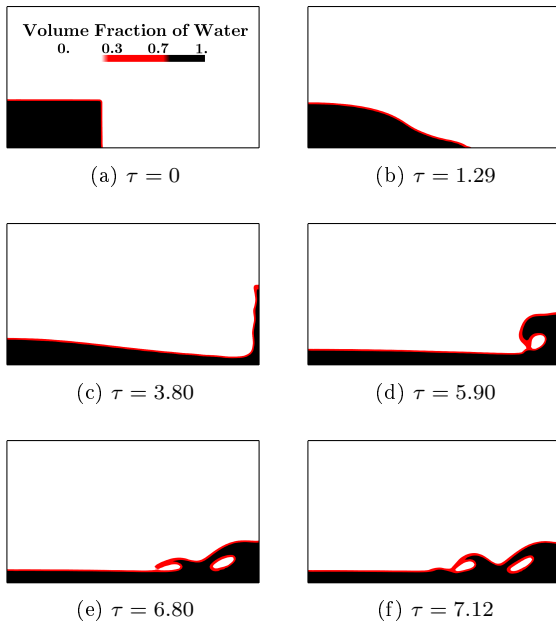


Figure 4: Dam-break simulation (a-f) temporal evolution of interface visualized in the form of volume-fraction contour. In the contour plots, a three color color-band is used to signify first regime, LSI regime and second regime using black, red and white color, respectively.

DAM BREAK SIMULATION

Simulation of classical dam-break scenario tests the capability of drag formulation of the LSI model to capture large scale interface under transient conditions. Physically, a water column confined to a corner of rectangular cavity as shown in Figure 3, is suddenly let off, triggering a dam break scenario wherein water rushes out to the other side of the cavity. Once the water body impacts the cavity wall, it rises along it till a certain height, after which it overturns and air is entrapped momentarily within the water body; during which the small as well as large scale interface co-exist.

The computational details of the test case are shown in Figure 3. A water column of width $1.2m$ and height $H = 0.6m$ is confined at bottom left corner of a cavity rectangular cavity of size $3.22m \times 1.8m$, filled with air. The top boundary of cavity is open to atmosphere and all other boundaries are set to wall. For this case, $k - \omega$ SST turbulence model is used for both the phases. A 2nd order TVD advection scheme is used for flow as well as volume-fraction equations. A uniform grid of size 144×80 is used here; considering the free fall velocity of the

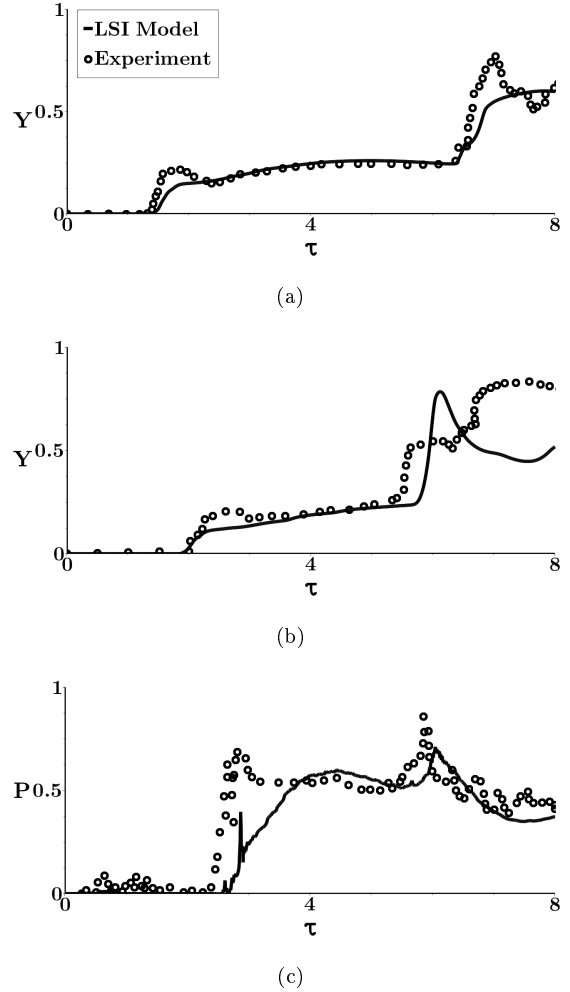


Figure 5: Comparison of temporal variation of non-dimensional interface height ($Y = y/H$) at plane (a) $H1$ and (b) $H2$ and (c) pressure ($P = p/\rho_1 g H$) calculated using the LSI model against the experimental results of Zhou et al., 1999. The non-dimensional time is defined as $\tau = t/\sqrt{H/g}$.

water column as velocity-scale, $u_s = \sqrt{2gH}$ and using conservative estimate of grid CFL number as 0.15, stable time-step value $\Delta t = 0.001s$ is used.

In the LSI model, water is taken as primary phase and air as secondary phase with threshold values of first regime terminus as 0.3 and second regime onset as 0.7. Three probes are used to collect temporal data i.e. the temporal variation of interface height at plane $H1$ and $H2$ as well as pressure at point $P1$, as shown in Figure 3. The variation of non-dimensional interface height ($Y = y/H$) and pressure ($P = p/\rho_1 g H$) with time ($\tau = t/\sqrt{H/g}$) are compared against the experimental results of Zhou et al., (1999).

Figure 4a-f, shows the temporal evolution of the interface visualized in the form of volume-fraction contour. Note that, the three color color-band signifies the first regime, LSI regime and second regime of the LSI model using black, red and white color, respectively. The plots show that, basic evolution of the water column, as reported in the experiment is captured reasonably well by the LSI model. Figures 4d-f show that, in addition to using interface drag in the vicinity of large scale interface, the LSI model uses first/second regime drag in the appropriate regions after the water overturns near the right

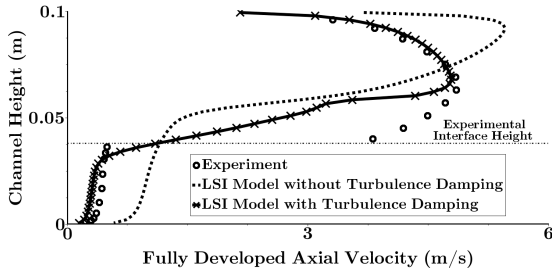


Figure 6: Comparison fully-developed mixture velocity (u_m) at $x = 9.1m$ predicted using the LSI model with and without turbulence damping against experimental results of Fabre et al., 1987.

wall of the cavity i.e. near the tip of the overturning water body and also in the region where air is entrapped. This flexibility of using different drag-law as a function of local topology in the LSI model provides the accuracy and robustness of solution. An animation (A1) of this case is also provided for reference.

The temporal variation of non-dimensional interface height at plane $H1$ and $H2$, shown in Figure 5a and b, respectively, show favorable comparison against experimental results. At both the locations, the time at which the first increase in interface height occurs is captured well; thereafter a monotonic increase is seen until the water body overturns and splashes back. The jump in the interface height is reasonably captured at both the locations with prediction at $H2$ over-predicting the time of steep rise. At later stages, there is increasing discrepancy with the experimental results, especially at plane $H2$; this may be due to the fact that numerically calculated values are merely average volume-fraction value at the respectively planes whereas experimental technique is not clear. In case of pressure, shown in Figure 5, there is less ambiguity between experimental as well as numerical measurement due to which better agreement is seen between the two results even at later stages.

TURBULENT AIR-WATER STRATIFIED FLOW

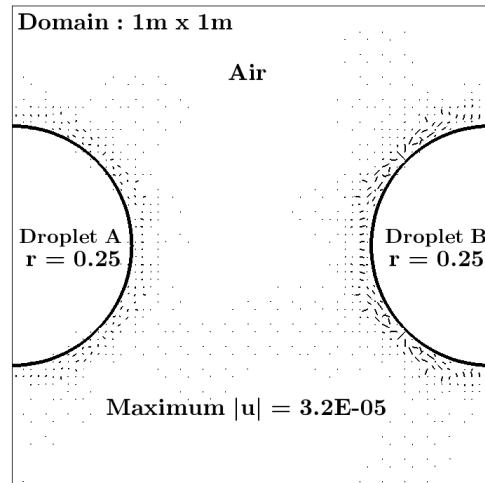
The role of LSI drag to predict stable and sharp interface for simulation of laminar stratified flow in a 2D channel was presented in our earlier study (Gada and Tandon, 2014). In the present work, turbulent air-water co-current stratified flow, studied experimentally by Fabre et al., (1987), is simulated using the LSI model.

Air and water enter the $12m$ long channel, $0.1m$ high and $0.2m$ deep at superficial velocity of $2.5m/s$ and $0.15m/s$, respectively with the interface being at $0.038m$ from bottom wall. The selected test corresponds to Run 250 of Fabre et al., (1987). In this particular case, 2D simulations are possible as the velocities are high enough for the interfacial friction to play an important role but 3D circulations are negligible.

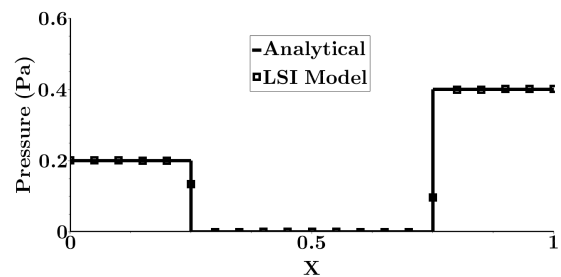
Simulations are done considering steady-state for a channel of size $12m \times 0.1m$ on a uniform 400×54 grid. $k - \omega$ SST turbulence model is used for both the phases with a couple of variations i.e. without and with turbulence damping near the large scale interface. In the latter case, the turbulence damping constant is taken as $T = 500$. A 2nd order TVD advection scheme is used for flow as well as volume-fraction equations.

From simulations, magnitude of fully-developed mixture velocity ($\vec{u}_m = \alpha_p \vec{u}_p + \alpha_s \vec{u}_s$) at $x = 9.1m$ from inlet is compared against experimental results of Fabre et al., (1987) in Figure 6. In the figure, experimental interface

height ($y = 0.038m$) is also shown to facilitate demarcation of two-phases. When the turbulence damping near the large scale interface is not used, there is inaccuracy even in the predictions near the physical walls. On using the turbulence damping, physically plausible results are seen. However, here too there is some discrepancy near the large scale interface, especially in the air side. The reasons for this difference in numerical results as compared to experiments needs further investigation. The implication of correct velocity field prediction is also seen in the pressure-drop prediction: with use of turbulence damping model the prediction improves from $17.40Pa/m$ to $2.86Pa/m$, which then compares reasonably with the experimental value of $2.1Pa/m$.



(a)



(b)

Figure 7: Young-Laplace law test (a) final interface shape and vector plot of mixture velocity signifying the magnitude of spurious currents (b) comparison of pressure along horizontal center-line against analytical solution.

YOUNG-LAPLACE LAW TEST

In the present work, a modified version of classical 2D Young-Laplace law test of Brackbill et al., (1992) is used where 2 fluid droplets (circular interface in 2D) of different fluids are used instead of a single fluid droplet. Initially, two infinite cylindrical rods of different fluids are placed in a quiescent surrounding fluid. Gravity and viscous forces are neglected, so surface tension force is balanced only by the pressure force. This results in pressure jump at the interface given by the Laplace equation $\Delta p = \sigma \kappa = \sigma/r$; the objective of this test is to evaluate ability of the surface tension module of the LSI model to determine this pressure-jump.

For simulation, a square computational domain of size $1m \times 1m$ is considered, shown in Figure 7a. Fluid rods, represented as a circle of radius ($r = 0.25m$) is initiated at a (0, 0.5) and (1, 0.5). Free-slip boundary condition is used at all boundaries. The density of the droplet A, droplet B and air is taken as $1280.84 kg/m^3$, $997.561 kg/m^3$ and $1.184 kg/m^3$, respectively. The coefficient of surface tension between air and droplet A is taken as $0.05 N/m$, whereas that between air and droplet B is taken as $0.1 N/m$. Simulations are carried out on 64×64 uniform grids with time-step $\Delta t = 10^{-5}$ till $t_{max} = 10\Delta t$.

Figure 7a shows the final interface shape as well as the mixture velocity vectors. The plot shows that interface has remained in equilibrium as pressure-jump balances the surface-tension forces maintaining the original circular shape. Moreover, the vector plot of the mixture velocity indicates the presence of spurious currents near the interface but its maximum value is quite small. Furthermore, Figure 7b shows the variation of pressure along horizontal center-line, in comparison against analytical solution. Clearly, the pressure variation across the two interfaces is free of any numerical oscillations and the magnitude of pressure-jump confirms to analytically obtained solution, the pressure-jump across the interface between air and droplet A should be $\Delta p = 0.2 N/m^2$ and that across the interface between air and droplet B should be $\Delta p = 0.4 N/m^2$.

SUMMARY

Model details of the Large Scale Interface (LSI) model implemented in the commercial code STAR-CCM+ are presented to simulate multi-scale multiphase flows within the multifluid model. The LSI model provides a general framework where three sub-topologies are defined for a pair of primary and secondary phases, based on volume-fraction of secondary phase into first regime, LSI regime and second regime. Within these sub-topologies, appropriate closure for momentum can be specified based on the problem at hand. Weighted sum of these individual closures forms the closure for the interaction between the phases. In the LSI regime, a drag law is used which can equalize the fluid velocities. In this regime, surface tension effects are also modeled. Additionally, for turbulent flows, a wall like damping treatment is done close to the large scale interface.

The LSI model is validated on three standard test cases; each case is selected to highlight the different capabilities of the LSI model. The simulation of classical dam-break scenario demonstrates the capability of drag formulation of the LSI model to capture large scale interface under transient conditions. Simulation of turbulent air-water co-current stratified flow shows the role of turbulence damping near the large scale interface, which proved critical to predict plausible pressure-drop value. The Young-Laplace law test showed that the LSI model predicts the analytically correct pressure profile, without significant spurious currents near the interface.

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