Informing the Development of multiphase CFD models using Bubbly Turbulent Flow Interface Tracking Results

L3:THM.ITM.P5.01 milestone report

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Abstract: Turbulent bubbly flow simulations were performed using interface tracking code, PHASTA, for a channel flow with Reynolds number of 400 (based on friction velocity) at 1% gas volume fraction. Another simulation using multiphase CFD approach (NPHASE-CMFD) code was performed for the same flow conditions. Statistical averaging of ITM results was used to determine certain model parameters for multiphase CFD approach (e.g. turbulent viscosity coefficient). It was demonstrated that informing the closure laws for multiphase flow model development by analyzing ITM results is a powerful tool for model development.
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1. Relevance to CASL and Objectives
For the development of the virtual reactor it is necessary to ensure high quality of the numerical modeling approach in all areas, including thermal hydraulics. It is well known that the two-phase flow modeling is essential for successful prediction of a wide set of challenge problems (e.g. DNS, CRUD). Multiphase CFD approach will play a major role in the VERA developed by CASL. In order to evaluate and improve the multiphase flow models implemented in CFD tools (such as Hydra-TH) employed in VERA, a finer scale simulations using interface tracking methods (ITM) are utilized to inform the development of multiphase CFD models.

In the presented report we will concentrate on the two-phase bubbly flow ITM results obtained by PHASTA code for an adiabatic air/water flow. We will perform detailed analysis of these results and extract turbulent viscosity information from the ITM data. A multiphase CFD code (NPHASE-CMFD) is used to demonstrate the modification of state-of-the-art CMFD model for the specific channel flow under consideration by comparing the results from the original and modified model formulations.

2. Description of numerical codes

PHASTA
PHASTA is a parallel, hierarchic, higher-order accurate (from the 2nd to the 5th order accuracy, depending on function choice), adaptive, stabilized (finite element) transient analysis flow solver (both incompressible and compressible). This approach has been shown by (Jansen, 1999) and (Whiting & Jansen, 2001) to be an effective tool for bridging a broad range of length scales in turbulent (RANS, large-eddy simulation (LES), detached eddy simulation (DES), DNS) flows. PHASTA (and its predecessor, ENSA) was the first unstructured grid LES code (Jansen, 1993) and has been applied to turbulent flows ranging from validation benchmarks (channel flow, decay of isotropic turbulence) to complex flows (airfoils at maximum lift, flow over a cavity, near lip jet engine flows and fin-tube heat exchangers). The PHASTA code uses advanced anisotropic adaptive algorithms (Sahni, et al., 2006) and the most advanced LES/DES models (Tejada-Martinez & Jansen, 2005). Note that DES, LES, and DNS are computationally intensive even for single phase flows. This capability has been recently (Nagrath, et al., 2006) extended to two phase flows where we use the level set method to track the boundary between two immiscible fluids (either compressible - where we captured new instabilities in sonoluminescence, or incompressible – to study bubble coalescence and two-phase turbulence (Bolotnov, et al., 2011)). PHASTA uses anisotropically adapted unstructured grids and its highly scalable performance on massively parallel computers has already been demonstrated (the code has shown good scaling out to 288*1024 IBM Blue Gene processors, at JUGENE, BG/P (Germany, #12 in top500 as of June 2011)), (Zhou, et al., 2010).

PHASTA is an open source code. However, in the current setup, it uses commercial linear solver libraries from Acusim, Inc. A possible switch to open-source solvers is considered (e.g. Trilinos, PETSc). Meshing capabilities utilize tools from Simmetrix, Inc. Creating mesh converters from open-source tools to PHASTA format is also a possibility. PHASTA works with hexahedral, tetrahedral and mixed meshes.
Governing Equations
The spatial and temporal discretization of the Incompressible Navier-Stokes (INS) equations within the FEM code PHASTA has been described in (Whiting & Jansen, 2001) and (Nagrath, et al., 2006). The strong form of the INS equations is given by:

Continuity: \[ u_{i,i} = 0 \]  \hspace{1cm} (1)

Momentum: \[ \rho u_{i,t} + \rho u_j u_{i,j} = -p_i + \tau_{i,j,j} + f_i \]  \hspace{1cm} (2)

For the incompressible flow of a Newtonian fluid, the viscous stress tensor is related to the fluid’s viscosity and the strain rate tensor as:

\[ \tau_{ij} = 2\mu S_{ij} = \mu (u_{i,j} + u_{j,i}) \]  \hspace{1cm} (3)

Using the Continuum Surface Tension (CST) model of (Brackbill, et al., 1992), the surface tension force is computed as a local interfacial force density, which is included in \( f_i \).

Level Set Method

The level set method of Sussman [(Sussman & Fatemi, 1999), (Sussman & Smereka, 1997), (Sussman, et al., 1999), (Sussman, et al., 1998)] and (Sethian, 1999) involves modeling the interface as the zero-level set of a smooth function, \( \varphi \), where \( \varphi \) is often called the first scalar and it represents the signed distance from the interface. Hence, the interface is defined by \( \varphi = 0 \). The scalar, \( \varphi \), is convected within a moving fluid according to,

\[ \frac{D\varphi}{dt} = \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0 \]  \hspace{1cm} (4)

where \( \mathbf{u} \) is the flow velocity vector. Phase-1, the liquid phase, is indicated by a positive level set, \( \varphi > 0 \), and phase-2, the gas, by a negative level set, \( \varphi < 0 \). Since evaluating the jump in physical properties using a step change across the interface leads to poor computational results, the properties near an interface were defined using a smoothed Heaviside kernel function, \( H_\varepsilon \), given by (Sussman, et al., 1999):

\[ H_\varepsilon(\varphi) = \begin{cases} 
0 & \text{if } \varphi \leq -\varepsilon \\
\frac{1}{2} \left[ 1 + \frac{\varphi}{\varepsilon} + \frac{1}{\pi} \sin \left( \frac{\pi \varphi}{\varepsilon} \right) \right] & \text{if } |\varphi| < \varepsilon \\
1 & \text{if } \varphi \geq \varepsilon 
\end{cases} \]  \hspace{1cm} (5)

The fluid properties are then defined as:

\[ \rho(\varphi) = \rho_1 H_\varepsilon(\varphi) + \rho_2 (1 - H_\varepsilon(\varphi)) \]  \hspace{1cm} (6)

\[ \mu(\varphi) = \mu_1 H_\varepsilon(\varphi) + \mu_2 (1 - H_\varepsilon(\varphi)) \]  \hspace{1cm} (7)

Although the solution may be reasonably good in the immediate vicinity of the interface, the distance field may not be correct throughout the domain since the varying fluid velocities throughout the flow field distort the level set contours (especially in fully resolved turbulent flow simulations). Thus, the level set was corrected with a re-distancing operation by solving the following PDE (Sussman & Fatemi, 1999):
\[ \frac{\partial d}{\partial \tau} = S(\varphi) \left[ 1 - |\nabla d| \right] \quad (8) \]

where \( d \) is a scalar that represents the corrected distance field and \( \tau \) is the pseudo time over which the PDE is solved to steady-state. This may be alternately expressed as the following transport equation:

\[ \frac{\partial d}{\partial \tau} + w \cdot \nabla d = S(\varphi) \quad (9) \]

The so-called second scalar, \( d \), is originally assigned the level set field, \( \varphi \), and is convected with a pseudo velocity, \( w \), where,

\[ w = S(\varphi) \frac{\nabla d}{|\nabla d|} \quad (10) \]

and \( S(\varphi) \) is defined as:

\[ S(\varphi) = \begin{cases} 
-1 & , \varphi < -\varepsilon_d \\
\varphi \left( 1 + \frac{1}{\pi} \sin \left( \frac{\pi \varphi}{\varepsilon_d} \right) \right) & , |\varphi| < \varepsilon_d \\
1 & , \varphi > \varepsilon_d 
\end{cases} \quad (11) \]

where \( \varepsilon_d \) is the distance field interface half-thickness which, in general, may be different from \( \varepsilon \) used in Eq. (5). Note that the zeroth level set, or interface, \( \varphi = 0 \), does not move since its convecting velocity, \( w \), is zero. Solving the second scalar to steady-state restores the distance field to \( \nabla d = \pm 1 \) but does not alter the location of the interface. The first scalar, \( \varphi \), is then updated using the steady solution of the second scalar, \( d \).

**NPHASE-CMFD**

NPHASE-CMFD (Antal, et al., 2000) is an advanced Computational Multiphase Fluid Dynamics computer code for the simulation and prediction of combined mass, momentum and energy transfer processes in a variety of single-phase (Gallaway, et al., 2008) and multiphase/multiscale systems, including gas/liquid (Wierzbicki, et al., 2007), (Tselishcheva, et al., 2010), solid/liquid (Tiwari, et al., 2006), (Tiwari, et al., 2009) and gas/solid/liquid (Antal, et al., 2000) flows. It uses two-phase k-\( \varepsilon \) models of turbulence (the user can chose between the high Reynolds number and low Reynolds number options of the model). The mixture and field continuity equations can be solved in a coupled or segregated (uncoupled) manner, using stationary coefficient linearization. The code is fully unstructured and can utilize second-order accurate convection and diffusion discretization. The technology used by the NPHASE-CMFD code is an ensemble averaged multifield model of two-phase or multiphase flows.

**Governing Equations**

A typical form of conservation equations for mass, momentum and energy, respectively, of interpenetrating fluids can be written as (Podowski, 2009):

\[ \frac{\partial}{\partial t} \alpha_k \rho_k + \nabla \cdot \alpha_k \rho_k \mathbf{V}_k = \Gamma_k \quad (12) \]
\[
\frac{\partial}{\partial t} \alpha_k \rho_k V_k + \nabla \cdot \alpha_k \rho_k V_k V_k = -\alpha_k \nabla p_k + \nabla \cdot \left[ \alpha_k (T_k + T_k^T) \right] \\
+ \alpha_k \rho_k g_k + (p_{ki} - p_k) \nabla \alpha_k - \nabla \alpha_k \cdot \mathbf{T}_{ki} + \mathbf{M}_k \\
\frac{\partial (\alpha_k \rho_k e_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{V}_k e_k) = -\nabla \cdot (\alpha_k \mathbf{q}_k) + \nabla \cdot \left[ \alpha_k (-\rho_k \mathbf{l} + \mathbf{F}_k) \cdot \mathbf{V}_k \right] + \alpha_k \rho_k \mathbf{g} \cdot \mathbf{V}_k + \xi_k \tag{13}
\]

where \( \alpha_k \) is the volume fraction of field-\( k \), \( \rho_k \) is the density of field-\( k \), \( \mathbf{V}_k \) is the velocity of field-\( k \), \( \Gamma_k \) is the mass transfer rate to field-\( k \), \( \bar{p}_k \) is the pressure in field-\( k \), \( \mathbf{T}_k \) is the total combined shear and turbulent shear stress for field-\( k \), \( \mathbf{q}_k \) is the gravity vector, \( \bar{\mathbf{g}}_k \) is the energy of field-\( k \), \( \mathbf{M}_k \) is the interfacial force per unit volume exerted on field-\( k \) by the other fields, and \( \xi_k \) is the corresponding interfacial energy transfer rate.

Whereas the interfacial mass transfer is directly related to the net heat transfer rate at the interface, the interfacial transfer of momentum and energy also involve the effects of interfacial pressure and shear stress.

In the case of gas/liquid bubbly flows, a two-field version of the above given model is used. In particular, the momentum conservation equations for the liquid (continuous field, ‘\( c \)’) and gas (dispersed field, ‘\( d \)’) can be written as

\[
\frac{\partial}{\partial t} \left[ (1-\alpha) \rho_c \mathbf{V}_c \right] + \nabla \cdot \left[ (1-\alpha) \rho_c \mathbf{V}_c \mathbf{V}_c \right] = -(1-\alpha) \nabla p_c + (p_c - p_c^i) \nabla \alpha \\
+ (1-\alpha) \nabla \cdot \mathbf{r}_c - (\tau_c - \mathbf{\tau}_c^i) \cdot \nabla \alpha + (1-\alpha) \rho_c \mathbf{g} + \mathbf{M}_c^i - \Gamma \mathbf{V}_c \tag{15}
\]

\[
\frac{\partial (\alpha \rho_d \mathbf{V}_d)}{\partial t} + \nabla \cdot (\alpha \rho_d \mathbf{V}_d \mathbf{V}_d) = -\alpha \nabla p_d - (p_d - p_d^i) \nabla \alpha + \alpha \nabla \cdot \mathbf{r}_d + (\mathbf{\tau}_d - \mathbf{\tau}_d^i) \cdot \nabla \alpha \\
+ \alpha \rho_d \mathbf{g} + \mathbf{M}_d^i + \Gamma \mathbf{V}_d \tag{16}
\]

where \( \alpha = \alpha_d \) is the local void fraction and \( \Gamma = \Gamma_d = -\Gamma_c \) is the local volumetric evaporation rate.

The model given by Eqs.(15)–(16) uses the Eulerian frame of reference and is based on the assumption that the individual fields can be treated as ‘equal partners’. However, it has been shown by Podowski (2009) that dispersed-gas/liquid flows do not follow, rigorously speaking, the interpenetrating-media concept. Fortunately, it has also been shown by (Podowski, 2009) that Eqs. (15) and (16) can still be used for gas/liquid flows, provided the following conditions are satisfied

\[
p_d = p_d^i = p_c = p_c^i = p \tag{17}
\]

\[
\tau_d = \mathbf{\tau}_d^i = \tau_c = \mathbf{\tau}_c^i = \tau \tag{18}
\]
**Interfacial momentum transfer**

Multifield ensemble-averaged models normally require several closure laws for the various interfacial transport phenomena. In particular, the interfacial momentum transfer can be determined by expressing the overall interfacial force as a superposition of the individual forces governing specific transport mechanisms between the fields:

\[
M_i^k = F_i^D + F_i^{VM} + F_i^L + F_i^{TD} + F_i^W
\]

where \( F_i^D \) is the drag force, \( F_i^{VM} \) is the virtual (added) mass force, \( F_i^L \) is the lift force, \( F_i^{TD} \) is the turbulent dispersion force and \( F_i^W \) is the wall force:

- **Lift force:**
  \[
  F_i^L = -C_L \alpha \rho_c \mathbf{V}_R \times \nabla \times \mathbf{V}_c \quad (20)
  \]

- **Turbulent dispersion:**
  \[
  F_i^{TD} = -C_{TD} \rho_c k_c \mathbf{V} \alpha \quad (21)
  \]

- **Wall force:**
  \[
  F_i^W = C_W \alpha \rho_c |\mathbf{V}_R||^2 \hat{\mathbf{n}}_W \quad (22)
  \]

- **Drag force:**
  \[
  F_i^D = -\frac{3}{4} \frac{C_D}{D_d} \rho_c |\mathbf{V}_R| \mathbf{V}_R \quad (23)
  \]

- **Virtual mass force:**
  \[
  F_i^{VM} = -C_{VM} \alpha \rho_c \left[ \frac{d\mathbf{V}_d}{dt} - \frac{d\mathbf{V}_c}{dt} \right] \quad (24)
  \]

**Turbulence modeling**

Another important modeling issue is concerned with two-phase flow turbulence. Typically, turbulence in multifield models used by CFD codes (such as Fluent, CFX, and others) is modeled using various versions of the \( k-\varepsilon \) model applied to the continuous field (Bertodano (1990), Anglart et al. (1997), Antal et al. (2000, 2003, 2005), Tiwari et al. (2006, 2009)). In the case of the commonly used \( k-\varepsilon \) model(s), the conservation equations for turbulent kinetic energy and energy dissipation can be written as

\[
\alpha_c \frac{Dk}{Dt} = \alpha_c \nabla \cdot \left( \frac{\nu^T}{\sigma_k} \nabla k \right) + \alpha_c \left( \frac{\nu^T}{\sigma_k} \nabla P_c - \varepsilon_c \right) \quad (25)
\]

\[
\alpha_c \frac{De_c}{Dt} = \alpha_c \nabla \cdot \left( \frac{\nu^T}{\sigma_c} \nabla \varepsilon_c \right) + \alpha_c \frac{\varepsilon_c}{k_c} \left( \frac{\nu^T}{\sigma_c} \nabla P_c - C_{1a} \varepsilon_c \right) \quad (26)
\]

where \( k \) is the turbulent kinetic energy, \( \varepsilon \) is the turbulent dissipation rate, \( \nu^T \) is the turbulent viscosity of the continuous (liquid) field, \( P_c \) is the rate of turbulent energy production.

The specific form of the expression for \( P_c \) depends on the particular version of the \( k-\varepsilon \) model, the High-Reynolds Number (High-Re) model (Jones & Launder, 1972) or the Low-Reynolds Number (Low-Re) model (Chien, 1982). The coupling between the turbulence model and the continuous-field
momentum conservation equation in single-phase flows is introduced via the continuous-field turbulent viscosity term, given by

\[ v_t = C_\mu f_\mu \frac{k^2}{\varepsilon_c} \]  

(27)

where \( f_\mu = 1 \) for the High-Re model and \( f_\mu = 1 - \exp(-0.0115 y^+) \) for the Low-Re model (Chien, 1982).

In the case of two-phase flows, the liquid-field turbulence may be augmented by the bubble-induced turbulence. The bubble-induced kinematic viscosity of the liquid phase can be determined from the model proposed by (Sato, et al., 1981)

\[ v_{\text{c}, k} = \sum_{k=1}^{N_d} C_{\mu b} d_{b,k} \alpha_k |\vec{v}_{\text{rel}, k}| \]  

(28)

where \( N_d \) is the number of dispersed fields, \( C_{\mu b} \) is the model coefficient, \( d_{b,k} \) is the average bubble diameter in the field-\( k \), \( |\vec{v}_{\text{rel}, k}| \) is the magnitude of the relative velocity of the field-\( k \). The Sato and Sekoguchi model has been successfully used before (Bertodano et al., 1990), but is important to recognize its limitations (in particular, as applied to non-bubble flows).

3. ITM-level Turbulent Bubbly Flow case design and Results

Here we describe the meshes for bubbly flow simulations performed by PHASTA.

For a smooth wall direct numerical simulation (DNS) we aim to resolve the turbulence fluctuations down to Kolmogorov’s scale. Typically mesh resolution is expressed in terms of viscous units, which are defined as:

\[ \Delta x_i^+ = \frac{u_i \Delta x}{v} \]  

(29)

where \( v \) is the kinematic viscosity, \( u_i \) is the friction velocity:

Figure 1. Simulation domain dimensions and axis orientation. Walls are shown as shaded areas.
Here $\tau_w$ is the wall shear stress and $\rho$ is the fluid density.

Table 1 summarizes the channel flow domain parameters. The mesh size used for the simulation is 21.4 million hexahedral elements.

### Table 1. Smooth wall simulation mesh parameters

<table>
<thead>
<tr>
<th>Direction</th>
<th>Boundaries</th>
<th>Number of nodes</th>
<th>Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>$0.0 \ldots 2\pi h$</td>
<td>587</td>
<td>$\Delta x^+ = 4.3$</td>
</tr>
<tr>
<td>y</td>
<td>$-1.0 h \ldots 1.0 h$</td>
<td>187</td>
<td>$\Delta y^+ = 4.3$</td>
</tr>
<tr>
<td>z</td>
<td>$0.0 \ldots \pi h$</td>
<td>195</td>
<td>$\Delta z^+ = 4.3$</td>
</tr>
</tbody>
</table>

Figure 1 shows a basic schematic of the computational domain. Periodic boundary conditions are applied in $x$ (stream-wise) and $z$ (span-wise) directions. Slip-velocity boundary conditions with appropriate wall shear is applied at the walls to ensure proper resolution of turbulent boundary layer.

Figure 2 shows the hexahedral mesh structure designed for the simulation.

The following procedure has been used to obtain the two-phase flow results:

- single-phase turbulent flow simulation is performed by applying the pressure gradient force to drive the flow which is based on the specified wall shear stress
- the single-phase data is analyzed and the steady-state conditions are obtained
- in the fully developed single-phase turbulence an initial distribution of bubbles is introduced by specifying an analytical expression for a distance field:
  \[ \varphi_i = \min_j \left( \left( x - x_j \right)^2 + \left( y - y_j \right)^2 + \left( z - z_j \right)^2 - R_i^2 \right) \]  \hspace{1cm} (31)
- two-phase simulation is advanced with both gravity and pressure gradient force. The sum of these forces acting on the two-phase mixture is equivalent to the desired wall shear stress
- the simulation is carried out to acquire sufficient fully-developed statistical data for bubble volume fraction and Reynolds stresses
Table 2. PHASTA mesh / simulation parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>( Re_\tau )</td>
<td>400</td>
</tr>
<tr>
<td>Number of fields</td>
<td>2</td>
</tr>
<tr>
<td>Number of bubbles</td>
<td>60</td>
</tr>
<tr>
<td>Void fraction</td>
<td>1%</td>
</tr>
<tr>
<td>Two-phase Reynolds number</td>
<td>29,530</td>
</tr>
<tr>
<td>Bubble diameter, ( D_b/\delta )</td>
<td>0.203</td>
</tr>
<tr>
<td>Eotvos number</td>
<td>0.110</td>
</tr>
<tr>
<td>Morton number</td>
<td>( 1.33 \times 10^{-11} )</td>
</tr>
<tr>
<td>Weber number</td>
<td>24.63</td>
</tr>
<tr>
<td>Number of elements</td>
<td>21.405 M</td>
</tr>
<tr>
<td>Mesh resolution in wall units:</td>
<td>4.3; 4.3; 4.3</td>
</tr>
<tr>
<td>Statistical sample size, non-dimensional time units:</td>
<td>5\times15</td>
</tr>
<tr>
<td>Number of computing cores used:</td>
<td>9,600</td>
</tr>
<tr>
<td>Elements per core:</td>
<td>2,230</td>
</tr>
</tbody>
</table>

Figure 3. Typical fully developed single-phase solution used to initialize the bubbly flow case.

Initial distribution of individual bubbles for the \( Re_\tau = 400 \) case is shown in Figure 4(a). Each bubble is resolved with 19 elements across diameter. The quality of this representation can be estimated from Figure 4(b). An example of instantaneous bubble distribution and liquid velocity field is shown in Figure 4(c).
Development of turbulent structures in the flow can be visualized by taking a contour of the normal-to-the-wall component of the vorticity of the instantaneous velocity field:

\[
(\nabla \times \mathbf{u})_y = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}
\]  

(32)

The resulting contours represent evolving 3D surfaces demonstrating the turbulence structures (such as hair-pin vorticities) developing in high-shear regions (near wall in turbulent channel). Different colors indicate a different direction of rotation (Figure 5).

Figure 4. Initial distributions of 60 bubbles (a) set by distance field initial condition for the moderate Reynolds number flow case. (b) quality of the bubble representation by a hexahedral mesh. (c) Turbulent bubbly flow simulation at time step 8,800. Instantaneous liquid velocity distribution is shown in planes with periodic boundary conditions and the bubble distribution is shown within the computational domain.
Figure 5. Turbulent bubbly flow simulation at time step 8,800. Bubbles and 3D contours of $y$-component of velocity curl are shown.

4. Advanced two-phase flow statistics of ITM simulations

A suite of averaging routines were developed to statistically analyze PHASTA results. A set of virtual probes were set-up in a single plane located at the downstream periodic boundary. The probe matrix size was 93 points across the channel ($y$, or normal-to-the-wall direction) by 42 points in the span-wise direction to allow for homogeneous direction averaging.

Two-phase flow statistics is obtained from raw ITM data using the following set of equations:

Mean velocity of phase-$k$:

$$U_k(t) = \frac{1}{\alpha_k n_e} \sum_{m=1}^{N_e} \left( \frac{1}{n_w} \sum_{j=1}^{N_w} X_k u_m^j (t + t_j) \right)$$ (33)

Volume fraction of phase-$k$:

$$\alpha_k(t) = \frac{1}{n_e} \sum_{m=1}^{N_e} \left( \frac{1}{n_w} \sum_{j=1}^{N_w} X_k (t + t_j) \right)$$ (34)

Turbulent kinetic energy of phase-$k$:

$$k_k(t) = \frac{1}{\alpha_k n_e} \sum_{m=1}^{N_e} \left( \frac{1}{n_w} \sum_{j=1}^{N_w} X_k \sum_{i=1}^{3} \frac{1}{2} \left( u_m^i (t + t_j) \right)^2 \right)$$ (35)
Turbulence dissipation rate:

$$\varepsilon^k(t) = \nu \left( \frac{1}{\alpha_k N_e} \sum_{m=1}^{N_e} \left( \frac{1}{N_w} \sum_{j=1}^{N_w} \sum_{i=1}^{3} \sum_{k=1}^{3} X_k \left( \frac{\partial u^i_m(t+t_j)}{\partial x_k} \right)^2 \right) \right)$$

(36)

Turbulent shear stress:

$$\tau_{xy}^k(t) = \frac{1}{\alpha_k N_e} \sum_{m=1}^{N_e} \left( \frac{1}{N_w} \sum_{j=1}^{N_w} X_k u^x_m(t+t_j) u^y_m(t+t_j) \right)$$

(37)

Relative velocity magnitude:

$$|V_{R\parallel}| = U^2_t - U^1_t$$

(38)

Mean strain rate tensor of phase-k:

$$\frac{\partial U^k_i}{\partial x_q}(t) = \frac{1}{\alpha_k N_e} \sum_{m=1}^{N_e} \left( \frac{1}{N_w} \sum_{j=1}^{N_w} X_k \frac{\partial u^l_m(t+t_j)}{\partial x_q} \right)$$

(39)

where $X_k$ is the phase indicator function for phase-$k$, $u^i_m(t+t_j) = u^i_m(t+t_j) - U^i(t)$ is the fluctuation of velocity component-$i$ computed during the ensemble run $m$ at the time instant $t + t_j$; $N_e$ is the number of ensemble runs, $N_w$ is the number of velocity samples in each window, $t$ is the current time, $t_j = (j - N_w/2) \Delta t$ is the local window time, and $\Delta t$ is the time step.

First, we analyzed fully developed single-phase flow results. Figure 6 shows the mean velocity (33), turbulent kinetic energy (35), and turbulent dissipation rate (36) profiles for the single-phase flow simulation.

Figure 6. Results of averaging of PHASTA data for a single phase run (Re$\tau$ = 400). Mean velocity (solid), turbulent kinetic energy (dashed) and absolute value of turbulent dissipation rate (dash-dot lines) are shown.
Evaluating turbulent viscosity constant based on ITM data

Statistics obtained in the previous section allows us to estimate the variation in turbulent viscosity in two-phase bubbly flows compared to single-phase counterpart:

- **turbulent viscosity:**
  \[ \nu_{T}^{DNS} = \tau_{xy} \frac{dU}{dy} \] (40)

**CMFD model information:**

- based on DNS data:
  \[ \nu_{T}^{k-\varepsilon} = C_{\mu} \frac{k^2}{\varepsilon}, \text{ where } k \text{ and } \varepsilon \text{ come from DNS data} \] (41)

- based on CMFD code results:
  \[ \nu_{T}^{CMFD} = C_{\mu} \frac{k^2}{\varepsilon}, \text{ where } k \text{ and } \varepsilon \text{ come from the solution of the equations} \] (42)

By obtaining the described statistics model constants can be adjusted to obtain better results (in this case \( C_{\mu} \) can be fitted). Since the \( k \) and \( \varepsilon \) distributions depend on the formulation of other terms in the R.H.S. of these equations, higher order statistics will be collected (production, diffusion terms) and term-by-term evaluation will be performed.

Note, that using Equations (40) and (41) one can estimate the value of the turbulent viscosity coefficient from DNS data:

\[ C_{\mu} = \frac{\tau_{xy}}{\frac{dU}{dy} k^2} \] (43)

Figure 7 shows the turbulent viscosity distribution obtained by averaging DNS data for single-phase channel flow (Eq. (40)). We compared this with Eq. (41) which shows the viscosity distribution while assuming the k-\( \varepsilon \) model expression and model constant value (\( C_{\mu} = 0.09 \)) is correct. Finally, we have extracted the value of \( C_{\mu} \) using equation (43). Note that for most of the channel the model-implied viscosity (dotted line) is larger than the DNS-extracted value (solid line). Also note that it is over predicted, as expected, near the wall where high-Reynolds number k-\( \varepsilon \) model is not applicable (the range of application is \( y^+ > 30 \)).

Based on the analysis of the single-phase DNS data, we would suggest to utilize the new value of \( C_{\mu}^{n} = 0.08 \). This observation is valid only for current simulation, and additional research should be done to demonstrate its applicability in a wider range of conditions.
5. CFD-level Turbulent Bubbly Flow case design and results

We have utilized NPHASE-CMFD code to re-produce the single and two-phase flow simulations which were performed by the ITM code, PHASTA. Note, that computational cost requirements for NPHASE are much lower than for PHASTA, as expected. In fact, the convergence of the single and two-phase solutions for simple channel flow geometries can be achieved within minutes for single-core runs compared to several 100,000 CPU hours in case of DNS/ITM approach.

NPHASE mesh / simulation parameters:

The overview of NPHASE-CMFD simulation parameters is given in Table 3. Note that High Reynolds number k-ε model requires the coarse resolution of $y^+ = 30$ at the wall. NPHASE is a finite-volume based code, and the solution is evaluated at cell centers. Thus, the resolution of $\Delta y^+ = 61$ was chosen for this specific case. Effectively 2D grid used for the NPHASE simulations is shown in Figure 8.

We have performed a base case simulation with default set of models and constants, described in NPHASE-CMFD model formulation (Section 2). NPHASE code used uniform inflow boundary conditions, and we observed a fully developed solution near the constant pressure outflow boundary ($x \sim 100$). Figure 9 and Figure 10 show the mean liquid velocity and gas volume fraction development in the NPHASE domain.
Table 3. NPHASE mesh / simulation parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re_τ</td>
<td>400</td>
</tr>
<tr>
<td>Number of fields</td>
<td>2</td>
</tr>
<tr>
<td>Void fraction</td>
<td>1%</td>
</tr>
<tr>
<td>Two-phase Reynolds number</td>
<td>29,530</td>
</tr>
<tr>
<td>Bubble diameter, D_b/δ</td>
<td>0.203</td>
</tr>
<tr>
<td>Domain size (x,y,z)</td>
<td>100×1×2π</td>
</tr>
<tr>
<td>Mesh size (x,y,z)</td>
<td>138×7×1</td>
</tr>
<tr>
<td>Number of elements</td>
<td>966</td>
</tr>
<tr>
<td>Mesh resolution in wall units:</td>
<td>100; 61; N/A</td>
</tr>
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<td>Number of computing cores used:</td>
<td>1</td>
</tr>
<tr>
<td>Elements per core:</td>
<td>3,120</td>
</tr>
</tbody>
</table>

Figure 8. Computational grid used in NPHASE-CMFD simulation (10x compressed in the stream-wise/horizontal direction).

Figure 9. Liquid velocity evolution in NPHASE-CMFD simulation.

We have investigated the effect of Sato two-phase viscosity modification, Eq. (28), on the bubbly turbulence modeling. For given conditions, the effect of applying the Sato viscosity is shown in Figure 11. We can observe that the effect of it is negligible on gas and liquid mean velocity profiles, but is more substantial on turbulent kinetic energy profile and gas volume fraction distribution.

We will use a base model without Sato viscosity to verify and improve the turbulence modeling constant based on the ITM results in the following section.
Figure 10. Gas volume fraction evolution in NPHASE-CMFD simulation.

Figure 11. NPHASE-CMFD results of two-phase bubbly channel flow simulations. Red plots correspond to no Sato contribution to turbulent viscosity, and black plots show the added Sato viscosity result. Gas mean velocity (black dash-dot and red dash-dot-dot), liquid mean velocity (solid and red dotted), turbulent kinetic energy in the liquid (dashed) and gas volume fraction (red long dash and black dotted lines) are shown.

6. Upscale of results to multiphase CFD level
The purpose of the detailed ITM study is to inform the development of multiphase CFD models. The following steps were described in the previous parts of this report:

- Perform the challenge simulations for turbulent multiphase bubbly flow (Part 3).
• Use state-of-the-art multiphase CFD model formulation to obtain the results for the same problem (Part 5)
• Advanced two-phase flow statistics was collected (Part 4).

In this part of the report we will use the results provided by Part 4 to modify the CMFD model formulation in Part 5 to obtain higher quality results. In particular, we will look into turbulent viscosity formulation, and modify the turbulent viscosity coefficient.

Both the original multiphase model formulation and modified version will be used to run the same case using two-fluid CMFD approach (e.g. NPHASE or other code if available) and compared with the averaged DNS results.

Single-phase channel flow analysis

The proposed approach of evaluating the turbulent viscosity coefficient from DNS and applying it to the CFD simulations was first tested for single-phase channel flow. As described in Part 4, the proposed value of $C_\mu$ based on DNS is 0.08. Figure 12 and Figure 13 show the results of NPHASE-CMFD simulations based on the original $C_\mu = 0.09$ and modified $C_\mu = 0.08$, respectively.

![Figure 12](image)

Figure 12. Comparison of PHASTA and NPHASE-CMFD results for single-phase channel flow ($C_\mu = 0.09$). PHASTA averaged results are shown in blue and NPHASE-CMFD results in red. Mean liquid velocity (solid), turbulent kinetic energy (short dashed) and absolute value of turbulent dissipation rates (long dashed lines) are shown.

There is a slight increase in predicted turbulent kinetic energy (dashed lines), but little change in turbulence dissipation rate (long dashed lines) and mean velocity profiles in comparison with ITM data provided (blue plots). However, due to non-linear coupling of $k$ and $\varepsilon$ equations and other modeling
assumptions (even the turbulent viscosity hypothesis itself) we do not achieve a perfect agreement. Note that we assumed a constant value of $C_\mu$ while the extracted distribution demonstrated substantial deviation from that value in Figure 7.

Figure 13. Comparison of PHASTA and NPHASE-CMFD results for single-phase channel flow ($C_\mu = 0.08$).

Two-phase bubbly channel flow analysis

In this section we will demonstrate the statistical averaging results of PHASTA two-phase flow bubbly simulations. Equations (33) - (36) were used to analyze the data from two-phase flow PHASTA simulations (Figure 5).

Figure 14 shows the mean liquid and gas velocity distributions across the channel along with turbulent kinetic energy and void fraction. Figure 15 shows the influence of 1% bubbles in the flow on the turbulent kinetic energy and turbulent dissipation rate distribution. Note that the most effect is in the $y' < 100$ region. This is an important observation in the framework of high-Reynolds number $k$-$\varepsilon$ models applied to two-phase flows since in this region boundary conditions for $k$ and $\varepsilon$ are usually specified. In order to obtain the turbulent viscosity distribution, mean shear and shear stress are extracted. Figure 16 show the comparison of these quantities for single and two-phase PHASTA simulations. Both simulations had the same pressure gradient applied which was balanced by wall shear. Naturally, the shear stress distribution is similar due to the same force balance. Finally, the extracted turbulent viscosity from the two-phase flow simulation is compared with the single-phase counterpart in Figure 17. While the statistical quality is not the best for this derived quantity, the overall distribution is close to the single phase case.
Figure 14. Mean liquid (solid blue) and gas (dash-dot) velocities, gas volume fraction (solid black) and turbulent kinetic energy (dashed line) distributions for 1% void fraction two-phase flow simulation using PHASTA ($Re_\tau = 400$).

Figure 15. Turbulent kinetic energy (solid lines) and turbulent dissipation rate (dashed lines) distributions based on PHASTA simulations for single (blue lines) and two-phase flows (red lines).
Figure 16. Mean velocity gradient (solid lines) and turbulent shear stress (dashed lines) distributions based on PHASTA simulations for single (blue lines) and two-phase flows (red lines).

Figure 17. Turbulent viscosity estimate using PHASTA simulations for single (solid line) and two-phase flows (long-dashed line).
Figure 18 demonstrated that the extracted values for $C_\mu$ are somewhat different for single- and two-phase flow cases. We would approximately estimate that 0.1 value is appropriate for two-phase modeling.

![Figure 18. Turbulent viscosity coefficient for single (dashed) and two-phase (dotted) flows based on PHASTA data analysis.](image)

**Averaged bubble drag coefficient estimate**

For two-phase flow simulation we utilized NPHASE-CMFD code and tested the effect of modifying turbulent viscosity coefficient ($C_\mu$) from 0.09 to 0.1 as well as adjusting the value of the drag coefficient from default 0.4 to 2.56. The latter value was derived using the balance between the buoyancy and drag forces: 

$$ (\rho_c - \rho_d) \alpha g - \frac{3}{4} C_D \frac{\alpha}{\rho_d} \rho_c |V_R| |V_R| = 0 $$

and the available DNS data.

The following table summarizes the set of 3 NPHASE-CMFD simulations described:

<table>
<thead>
<tr>
<th>Case name</th>
<th>$C_\mu$</th>
<th>$C_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.09</td>
<td>0.4</td>
</tr>
<tr>
<td>B</td>
<td>0.09</td>
<td>2.56</td>
</tr>
<tr>
<td>C</td>
<td>0.1</td>
<td>2.56</td>
</tr>
</tbody>
</table>

The following series of plots demonstrates the effects of informing the constants in CMFD model. Figure 19 shows that the relative velocity agreement dramatically improves after the change in drag
coefficient. Liquid velocity discrepancy near the center line can be explained by poor prediction of void fraction distribution in this region (Figure 20).

Figure 19. Mean liquid (red) and gas (blue) velocities based on PHASTA results (solid), NPHASE case A (dotted), case B (dashed) and case C (symbols) simulations.

Figure 20. Gas volume fraction distribution based on PHASTA results (solid), NPHASE case A (dotted), case B (dashed) and case C (symbols) simulations.
Figure 21 demonstrates the improved prediction of turbulent kinetic energy when modifying the drag coefficient. Turbulence dissipation does not heavily depend on the modified parameters (Figure 22).

**Figure 21.** Turbulent kinetic energy distribution based on PHASTA results (solid), NPHASE case A (dotted), case B (dashed) and case C (symbols) simulations.

**Figure 22.** Turbulent dissipation rate distribution based on PHASTA results (solid), NPHASE case A (dotted), case B (dashed) and case C (symbols) simulations.
Finally, we can observe a significant improvement in the turbulent viscosity prediction (Figure 23).

![Turbulent viscosity distribution](image)

**Figure 23. Turbulent viscosity distribution based on PHASTA results (solid), NPHASE case A (dotted), case B (dashed) and case C (symbols) simulations.**

7. Future Work

The described techniques can be immediately applied to various flow rates, void fractions and fluid parameters to evaluate the turbulence modeling approach on a wider scale. Future applications may include:

- analysis of boiling flows, and detailed studies of turbulence modification by growing nucleating bubbles near the wall, and condensing bubbles near the centerline for subcooled boiling
- study of low Reynolds number models with resolved walls and development of advanced CMFD models
- evaluation of advanced turbulence models and their inherent abilities to predict two-phase flow phenomena.

Advance upscaling techniques will be developed to utilize the ITM capabilities in CMFD model development. In particular, the improvement and validation of interfacial forces is an important direction. For fully developed steady-state simulations of vertical two-phase flows the following interfacial force balance equations should be satisfied:
Wall-normal balance:
\[
F_k^L + F_d^{TD} + F_d^W = 0
\]

\[
-C_L \alpha \rho_c \nabla \times V_R - C_{TD} \rho_c k_c \nabla \alpha + C_W \alpha \rho_c |V_R||^2 \hat{n}_W = 0
\] (44)

Stream-wise vertical balance:
\[
F_d^B + F_d^B = 0
\] (45)

\[
(\rho_c - \rho_d) \alpha g - \frac{3}{4} C_D \frac{\alpha}{D_d} \rho_c |V_R| V_R = 0
\]

Based on averaged ITM data we can obtain:

\[
F(y) = F_k^L + F_d^{TD} + F_d^W = -C_L \alpha \rho_c V_R \times \nabla \times V_c - C_{TD} \rho_c k_c \nabla \alpha + C_W \alpha \rho_c |V_R||^2 \hat{n}_W
\] (46)

\[
F(x) = F_d^B + F_d^B = (\rho_c - \rho_d) \alpha g - \frac{3}{4} C_D \frac{\alpha}{D_d} \rho_c |V_R| V_R
\] (47)

In order to evaluate these expressions the following information is needed:

- void fraction, \( \alpha \)
- turbulent kinetic energy, \( k_c \)
- \( V_R \times \nabla \times V_c \) can be approximated as \( U_R \frac{\partial U_c}{\partial y} \) for channel flows
- relative velocity, \( |V_R| \)

**Bibliography**


