Influence of Inlet Turbulent Boundary Conditions on Bubble Diameter Calculation

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1. Introduction

Bubble hydrodynamics plays a crucial role in various industrial applications, especially in nuclear safety where the accurate determination of bubble size is significant. One of the key applications is pool scrubbing, a process that removes aerosol fission particles from gas bubbles to depressurize the containment of a nuclear reactor during accidents. The ratio between the injected and escaped mass from the pool, the De-contamination Factor (DF), is commonly used to evaluate the effectiveness of pool scrubbing.

Traditionally, pool scrubbing calculation relied on empirical correlations to estimate bubble diameter, but this method has limitations and can result in an inadequate estimation of the DF. Mechanistically modeled approaches, such as the Interfacial Area Transport Equation (IATE), can improve the prediction capabilities by dynamically estimating bubble diameter through breakup and coalescence mechanisms. However, most IATE models were developed for fully developed pipe flow conditions and may not be suitable for the recirculation flows in a large tank or pool that is typically found in pool-scrubbing gas-liquid flow conditions.

To accurately predict such flow behaviors, a multidimensional approach is necessary through advanced turbulence and transport modeling. Especially, turbulence modeling is a critical aspect of correctly predicting bubble diameter. The calculation of turbulent kinetic energy and energy dissipation rate in the flow is necessary to model the breakup and coalescence mechanisms that contribute to bubble diameter calculation. Therefore, accurate determination of the turbulent boundary conditions at the inlet is crucial. For this reason, this paper investigates a method for imposing the appropriate inlet turbulent boundary conditions at pool scrubbing conditions to accurately calculate the bubble diameter. By using a Computational Fluid Dynamics (CFD) code together with IATE, it is aimed to provide a more accurate prediction of the mean bubble diameters at pool scrubbing conditions.

2. Methodology and Results

This paper focuses on accurately determining the bubble size in pool scrubbing, a process involving the movement of multiple phases within a pool or pipe. The Sauter Mean Diameter (SMD) reported in a recent study by Yoshida et al. [1] will be evaluated using IATE with the OpenFOAM code. The determination of inlet turbulent boundary conditions, such as turbulent kinetic energy and energy dissipation rate, is crucial to estimating turbulence parameters in the domain. However, the general method of determining boundary conditions may not be suitable for certain pool scrubbing conditions. In the following sections, the details of turbulence modeling, boundary conditions, and bubble diameter calculation will be discussed.

2.1 Turbulence Modelling in General

Turbulence modeling simplifies solving turbulent flows by transforming the flow using average flow variables, which significantly reduces computational time. Reynolds Decomposition is used to obtain these mean flow variables, where the instantaneous velocity is assumed to be the sum of the mean spatial and turbulent fluctuation velocity. This can be applied to pressure and velocity equations, resulting in the Reynolds Averaged Navier-Stokes (RANS) equations. The RANS equations include an additional term, the Reynolds stress tensor, which needs to be determined through turbulence modeling. Eddy viscosity models are commonly used to solve this problem. Eddy viscosity models estimate the Reynolds stress by relating the shear stress from the eddies to the shear stress from the mean flow. The Reynolds stress is calculated using a proportionality constant called dynamic turbulent viscosity. Thus, one can close the governing equations after obtaining the Reynolds stress by modeling the turbulent viscosity. The $k-\varepsilon$ model uses two transport equations for turbulent kinetic energy, k, and turbulent energy dissipation rate, ε, to estimate the turbulent viscosity, μ_t. The relationship between these parameters is given by Equation (1). As can be seen in Eq. (1), once the k and ε are estimated the turbulent viscosity can be calculated. Using this relationship, a constraint will be proposed to estimate boundary values of k and ε.

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \rightarrow \nu_t = C_\mu \frac{k^2}{\varepsilon} \quad [k-\varepsilon] \tag{1}$$

Bubble Induced Turbulence (BIT) or pseudo-turbulence refers to velocity changes caused by the movement of liquid as bubbles penetrate through it. BIT is different from Shear Induced Turbulence (SIT), which does not account for the wake effects of bubbles in the turbulence intensity. BIT considers how the dispersed phase affects the turbulence in the continuous phase. To account for the effects of BIT in $k-\varepsilon$ models, additional source terms can be added to the k and ε transport equations.

2.2 Turbulence Modelling in OpenFOAM

In OpenFOAM, a solver is a computational algorithm that solves the governing equations of a fluid flow problem. The *multiphaseEulerFoam* solver was selected for this study as it can handle a system of many compressible fluid phases and is commonly used for two-phase simulations. Among several turbulence models, the *mixtureKEpsilon* model is selected as the RANS model in this study considering it allows for different turbulence characteristics in each phase and accounts for the effect of the dispersed phase on the turbulence of the continuous phase. Unlike other RANS models, the *mixtureKEpsilon* considers the effect of the disperse phase and uses mixture properties instead of only liquid, making it suitable for higher void fraction flows. The model is a two-equation model for k and ε and was theorized by Behzadi et al [2] as given in Eq. (2) where m relates to the mixture of the two phases. The BIT can be included by introducing additional source terms to the k and ε transport equations as $S_{k,m}$ which is shown in Eq. (2). The model coefficients C_1, C_2, C_3, σ_k and σ_ε varies depending on the flow conditions.

$$\begin{aligned}\frac{\partial(\rho_m k_m)}{\partial t}+\nabla\cdot(\rho_m \boldsymbol{U_m} k_m) &= \nabla\cdot\left[\left(\mu_{MOL}+\frac{\mu_{m-SIT}}{\sigma_k}\right)\nabla k_m\right]+P_{k,m}-\rho_m\varepsilon_m+S_{k,m}\\ \frac{\partial(\rho_m \varepsilon_m)}{\partial t}+\nabla\cdot(\rho_m \boldsymbol{U_m} \varepsilon_m) &= \nabla\cdot\left[\left(\mu_{MOL}+\frac{\mu_{m-SIT}}{\sigma_\varepsilon}\right)\nabla \varepsilon_m\right]+\frac{\varepsilon_m}{k_m}(C_1 P_{k,m}-C_2\rho_m\varepsilon_m)+C_3\frac{\varepsilon_m}{k_m}S_{k,m}\end{aligned} \quad (2)$$

The mixture equations in bubbly flow tend to continuous phase due to mass averaging when the density of the continuous phase is much greater than that of the dispersed phase. To improve the BIT modeling, OpenFOAM implemented an effective density for the gas ($\rho_{g-eff}=\rho_g+C_{vm}\rho_l$) using the virtual mass coefficient and the liquid density in the averaging and an alternative model for bubble-generated turbulence. The bubble-generated turbulence in the *mixtureKEpsilon* model of OpenFOAM is implemented using the Lahey [3] model, which calculates an additional source term as a function of the interfacial drag coefficient, C_D, the velocity difference ($\mathrm{U_r}=\mathrm{U_l}-\mathrm{U_g}$) between the liquid and gas phase, void fraction, α_g, and the bubble diameter, $\mathrm{D_b}$, as shown in Eq. (3).

$$S_{k,m}=\frac{k_{\mathrm{cl}}}{C\varepsilon_2\varepsilon_{\mathrm{cl}}}S_\varepsilon=C_p\left(1+C_{\mathrm{D}}^{4/3}\right)\alpha_{\mathrm{g}}\frac{|U_r|^3}{D_{\mathrm{b}}} \quad (3)$$

Table I shows two additional coefficients, $\mathrm{C_p}$ and α_p, in comparison to the standard $k-\varepsilon$ model. The C_p coefficient, which is a model constant for bubble-generated turbulence, is given as 0.25 by Arnold et al. [3] but taken as 0.1 in this study considering non-spherical shaped bubbles. OpenFOAM has additionally implemented α_p to control the gas phase fraction and exclude bubble-generated turbulence in domains with high void fractions. The values of C_p and α_p should be determined based on the flow and geometrical conditions. The details of the implementation of the *mixtureKEpsilon* model are available in [2] and [3].

Table I: mixtureKEpsilon Coefficients

	C_μ	C_1	C_2	C_3	C_p	α_p	σ_k	σ_ε
Value	0.09	1.44	1.92	C_2	0.25	0.3	1.0	1.3

2.3 Initial and Boundary Conditions

OpenFOAM is a collection of C++ libraries used for solving continuum mechanics problems through the Finite Volume Method (FVM). A case directory is required, containing 0, constant, and system folders, each with different contents like initial/boundary conditions, mesh and phase properties, solver and system settings. The initial and boundary conditions of the turbulent kinetic energy, k, and energy dissipation, ε, must be accurately provided for the air, water, and mixture since they affect the entire solution. Despite its importance, there is no direct method to estimate these inlet conditions since the flow conditions differ. Two practical methods for estimating turbulent viscosity are Turbulent Intensity (Ti) and Viscosity Ratio (VR). Ti is the ratio of velocity fluctuations to mean velocity, while VR is the ratio of turbulent viscosity to molecular viscosity. Since these values are unknown at the inlet, it's challenging to estimate boundary conditions using either method. Therefore, a pre-determined Ti or Vr is typically used. This study will use Ti, and a general method for estimating inlet k and ε is given below.

1. Determine the Characteristic Length: $\mathrm{L_c}$
2. Calculate the Mixing Length: $\mathrm{L_m}=0.07\mathrm{L_c}$
3. Calculate the Reynolds Number: $\mathrm{Re}=\frac{\mathrm{UL_c}}{\nu}$
4. Calculate the Turbulent Intensity: $\mathrm{T_i}=0.16\mathrm{Re}^{-1/8}$
5. Calculate the Turbulent Kinetic Energy: $k_{in}=\frac{3}{2}(UT_i)^2$
6. Calculate the Energy Dissipation Rate: $\varepsilon_{in}=C_\mu^{3/4}\frac{k_{in}^{3/2}}{L_m}$
7. Calculate the Turbulent Viscosity: $\nu_t=C_\mu\frac{k_{in}^2}{\varepsilon_{in}}$

Following the list above it can be seen that determining a characteristic length is a crucial parameter to calculate various fluid flow properties. The characteristic length is based on the geometry of the system and it may be different for different applications such as the diameter of the pipe in a pipe flow, the hydraulic diameter in a duct, the nozzle or column diameter for a bubble column reactor, and the chord length of the wing in an aircraft wing flow. After determining the characteristic length, the mixing length, which describes the size of eddies or turbulent structures in a fluid flow, can be calculated. It should be noted that the used empirical mixing length correlation is for fully developed turbulent pipe flows. Since now the characteristic length is known the Reynolds number can be calculated using the inlet velocity and the molecular kinematic viscosity. After calculating the Reynolds number, the Ti can be found using the correlation on the list. Turbulence levels are considered low if $\mathrm{T_i}\leq 1$, moderate $1<\mathrm{T_i}\leq 5$, and high $5<\mathrm{T_i}\leq 20$). The Ti

correlation on the list is only applicable for fully developed turbulent pipe flows. After finding the Ti, the inlet turbulent kinetic energy can be calculated using the inlet velocity. Finally, the energy dissipation can be estimated using the turbulent kinetic energy and a standard $k-\varepsilon$ constant, $C_\mu = 0.09$. Turbulent kinetic energy and energy dissipation rate can be estimated as described above, but the correlations used may not be suitable for pool scrubbing flow conditions. It is possible to assume a Ti value directly, but the generally adopted values (3 to 5%) may also not be suitable for pool scrubbing conditions. Therefore, another method must be developed to determine Ti in such conditions. To calculate the fictitious turbulent viscosity accurately, one approach could be to consider the order of molecular kinematic viscosity. The calculated inlet turbulent viscosities can be verified by constraining them to the ranges of the molecular viscosities which can be obtained from the fluid properties.

2.4 Turbulent Intensity Estimation

Yoshida et al. [1] conducted an experiment to report on SMD for several cases involving air injection into still water. They used a Wire Mesh Sensor (WMS) to measure gas void fraction and velocities at various depths in a 0.5 m x 0.5 m square channel with a 1 m submergence and a 10 mm single inlet nozzle. Assuming the nozzle diameter as the characteristic length and using the Pipe Flow Approach (PFA) and Molecular Viscosity Approach (MVA), the inlet boundary conditions can be obtained as shown in Table II.

Table II: mixtureKEpsilon Coefficients

Method	L_c [m]	Re [-]	L_m [m]	T_i [%]	k_{in} [m^2/s^2]	ε_{in} [m^2/s^3]	ν_t [m^2/s]
PFA	0.01	4215.36	0.0007	5.64	1.934E-01	1.996E+01	1.686E-04
MVA	0.01	-	0.0007	0.51	1.554E-03	1.437E-02	1.511E-05

The MVA approach utilizes the correlation for Ti from Step 4 as an initial estimate and iteratively computes the Ti when molecular viscosity equals turbulent viscosity. The resulting Ti is 0.51%, whereas using PFA would result in a larger Ti of 5.64% as can be seen in Table II. This indicates that employing the standard PFA instead of MVA could cause the system to have an order of magnitude larger turbulent viscosity and Ti. Without reported inlet turbulence parameters in the Yoshida experiment, it is challenging to determine the appropriate Ti. Nonetheless, examining the typical values of Ti in other bubble column experiments could provide some insights. In the Akbar et al. [5] experiments, most inlet Reynolds numbers are in the laminar range, with the highest in the transitional range. The reported mean fluctuation velocity can be used to estimate Ti at the inlet and domain, by dividing it by orifice and bulk velocities, respectively. Results show lower Ti at the inlet due to lower bulk velocity than high injection inlet velocity. The Yoshida experiment also has a similar trend, with high inlet velocity air injected into still water at a Reynolds number of 4215.36, which is at the higher end of the transitional flow. Therefore, turbulent viscosity can be closer to molecular viscosity than much higher values typically assumed in CFD calculations.

2.5 Simulation

The Eulerian-Eulerian simulations of the Yoshida et al. [9] experiment will be simulated for 20 seconds using OpenFOAM-V10 from the OpenFOAM Foundation©. The *multiphaseEulerFoam* solver will be used on pure hexahedron meshes with 393,260 elements and a maximum 1.12867 aspect ratio for the test section. Interphase exchange is explicitly modeled due to averaging in Eulerian simulations resulting in loss of interphase details. The momentum conservation equation is used for closure modeling of interfacial forces including Drag, Lift, Turbulent Dispersion, and Virtual Mass. OpenFOAM can employ these interfacial models separately for the dispersed and continuous phases. One-group IATE will be used for the simulation to estimate SMD (d_{sm}) which can be calculated through interfacial area curvature, κ, as shown in Eq. (4). It can be seen in the equation that κ is the ratio between the Interfacial Area Concentration (IAC) and the void fraction. It should be noted that the mechanistic modeling of one-group IATE is largely based on fully developed pipe flow and differs from pool flow.

$$D_b \equiv d_{sm} = 6\frac{\alpha}{a_i} \;\rightarrow\; D_b \equiv d_{sm} = \frac{6}{\kappa} \qquad (4)$$

Table III presents a simulation matrix created with the MVA approach described earlier. The Ti was calculated at a turbulent viscosity equal to molecular viscosity to determine the inlet turbulent boundary conditions. Varying Ti from 1 to 20 percent, corresponding inlet turbulent k and ε were obtained to study their effect on bubble diameter. The simulation matrix in Table III can be used with the one-group IATE to guide setting inlet boundary conditions for pool scrubbing conditions.

Table III: Simulation Matrix

T_i [%]	k_{in} [m^2/s^2]	ε_{in} [m^2/s^3]	ν_t [m^2/s]
0.51	1.55344E-03	1.43723E-02	1.51114E-05
1.00	6.08654E-03	1.11465E-01	2.99119E-05
3.00	5.47788E-02	3.00956E+00	8.97356E-05
5.00	1.52163E-01	1.39331E+01	1.49559E-04
10.00	6.08654E-01	1.11465E+02	2.99119E-04
20.00	2.43461E+00	8.91721E+02	5.98238E-04

2.6 Results

The Void fraction, Air and Water Velocities, and SMD results for a diagonal cut of the domain are shown in Fig. 1, demonstrating typical bubble column behavior with the highest velocities in the transitional regions from jet to swarm. Fig. 2 presents time-averaged void fraction and turbulent kinetic energy profiles at 100, 500, and 900 mm. The void fraction profile disperses toward

downstream as expected, however, a direct comparison with the experimental data is not possible because Yoshida et al. did not report void fraction profiles. The effect of higher Ti is visible in higher velocity areas, particularly in the transitional regions where the peak turbulent kinetic energy is highest.

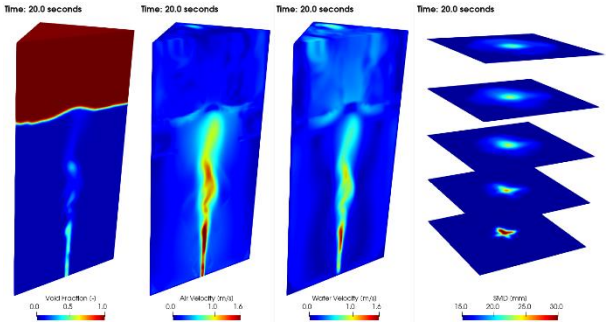

Fig. 1. Void Fraction, Velocities, and SMD

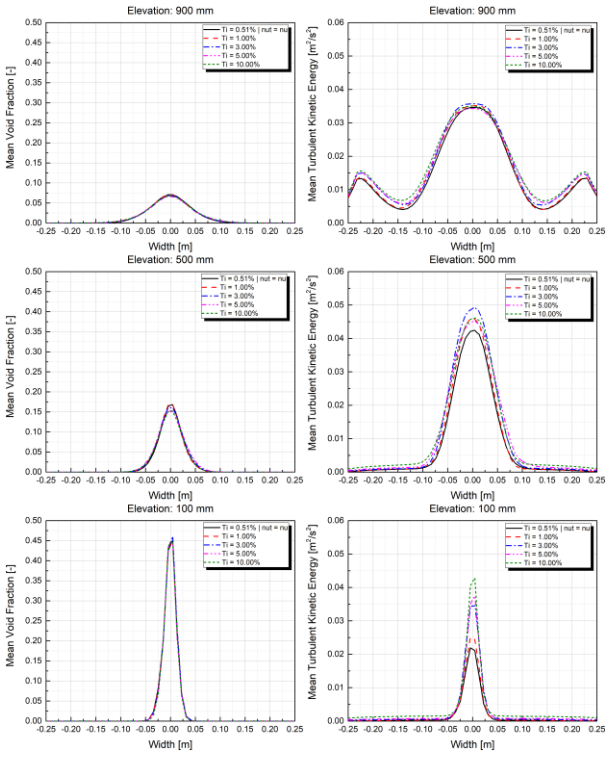

Fig. 2. Mean Void and Turbulent Kinetic Energy

Fig. 3 compares the SMD with experimental results except for the 20% Ti case since the simulation crashed. The best agreement is obtained when the turbulent viscosity is close to the molecular viscosity, indicating that the commonly used 3-5% Ti values are too high for pool scrubbing conditions. The discrepancy between the simulation and experimental increases in the swarm region due to IATE breakup and coalescence. To improve results at higher elevations, a higher IAC is needed to decrease SMD values.

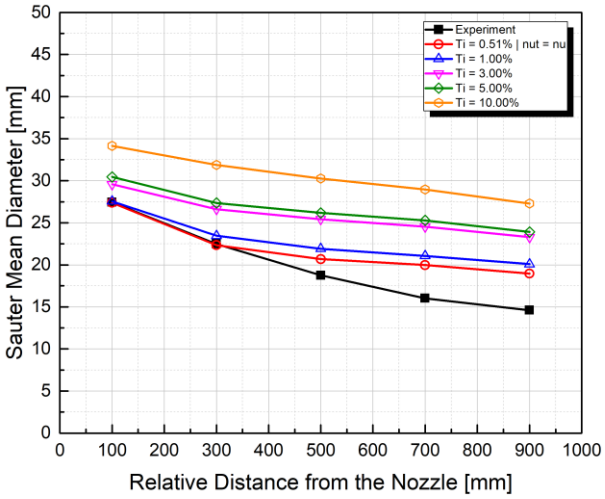

Fig. 3. Turbulent Viscosity Effect on SMD

3. Conclusions

The study examined the influence of inlet turbulent boundary conditions on bubble diameter under pool scrubbing conditions. Results revealed that Ti could be estimated differently based on whether the flow at the inlet is laminar, transitional, or turbulent. If the flow is laminar or transitional, turbulent viscosity can be assumed to be similar to molecular viscosity, resulting in lower Ti (< 1%). On the other hand, if the flow is turbulent at the inlet, then the turbulent viscosity can be assumed to be larger than molecular viscosity, and the resulting Ti is similar to that of pipe flow (1-5%).

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