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Numerical simulation of a square bubble column using Detached Eddy Simulation and Euler–Lagrange approach

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To accurately simulate industrial sized bubble columns, the accurate prediction of the turbulent structures is important. Currently used RANS and LES models cannot capture the dynamics of the bubble columns or require a high grid resolution, respectively. In this work the Detached Eddy Simulation (DES) was used to combine the advantages of RANS and LES approaches. The DES method was based on Spalart–Allmaras, k–ε and k–ω SST turbulence models and was used to simulate gas–liquid flow for a bubble column with a square cross-section. The results are compared with experimental data and Large Eddy Simulation (LES) results, based on the Vreman and Smagorinsky subgrid-scale models. Profiles of turbulence kinetic energy and average axial liquid and gas velocities are compared at three heights of the column: near the sparger, in the middle and at the top of the column. The obtained results are in a very good agreement with the experimental data and LES simulations, proving ability of DES to capture highly dynamic flow motion and accurately predict main liquid characteristics in gas–liquid systems.

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1. Introduction

Bubble column reactors (BCR) are considered to be a very versatile and efficient type of reactor in many chemical and biochemical processes, such as: Fisher–Tropsch process, waste water treatment and absorption. Despite its simplicity, a successful design and scale-up of BCRs requires a detailed understanding of multiphase fluid and gas dynamics, which can be obtained using (combined) experimental and numerical approaches, see Table 1.

Because of the complex flow patterns and the high void fraction it is often difficult to determine the main liquid and gas characteristics experimentally. In large-scale systems, like pilot or industrial plants, non-intrusive techniques are not capable to capture the dynamics of the flow in the bulk, due to the opacity of the liquid. While intrusive techniques might increase perturbations of the flow and as a result, influence the data (Roghair, 2013).

To overcome limitations of physical experiments, numerical approaches are frequently used for a detailed investigation of BCRs. Despite theoretical boundless abilities of numerical techniques, the simulation of industrial (large scale) BCRs still passes a huge challenge, due to limits in available computational power, quality of closures and models capabilities (Spalart, 2000). Moreover, large scale BCRs are determined by large amount of gas (and/or solid) inclusions, which induces turbulence motion on multiple scales and therefore increases complexity of the physical description of the system even more.

The most frequently used technique for industrial scale simulations of two-phase gas–liquid flows is the Euler–Euler (E–E) approach, which represents the continuous liquid phase and bubbles as interpenetrating fluids. This approach has been proved to be suitable for industrial applications, due to its relatively low computational power requirements (Xiaoping et al., 2017). However, the method demands for careful formulation and treatment of closures for phases interactions and loses information on the scale of the individual bubble. As a result it is difficult to take into account break-up or coalescence.

As an alternative, the Euler–Lagrange (E–L) approach with direct tracking of the dispersed gas phase may be used. The most popular method is the Discrete Bubble Modeling (DBM), which explicitly treats the bubble–bubble interaction. However, this deterministic E–L approach is computationally intensive and thus, can not be scaled up toward industrial scales (Darmana, 2006).

It is of big interest to develop and investigate methods for large-scale systems which will allow to keep bubbles as individual objects. Based on the E–L method, Kamath et al. (2017) proposed...
to use Direct Simulation Monte Carlo (DSMC) as an alternative to DBM. The stochastic nature of DSMC handles bubble-bubble collisions more efficiently in comparison to deterministic DBM. Thus, the method can in principle be applied to a much larger amount of bubbles.

Since bubble dynamics is directly coupled with dynamics of the surrounding liquid it is very important to have a suitable method for resolution of complex turbulent flows at large scales. Generally, simulations of large-scale systems are based on Reynolds-Averaged Navier−Stokes (RANS) equations in combination with the E−E approach (Laborde-Boutet et al., 2009), primarily because of the low grid density requirements of RANS models in most areas of the computational domain. However, the time-averaged nature of RANS equations does not allow for an accurate representation of highly dynamic flows in bubble column reactors. Therefore, they may give only rough estimates of the key hydrodynamic parameters. In addition, the semi-empirical nature of most RANS models limits the area of their applicability, since internal constants were calibrated only for a particular type of single-phase flows.

The more accurate method for turbulence modeling of BCRs is Large Eddy Simulation (LES), which resolves large-scale turbulent eddies and models unresolved turbulence using subgrid-scale (SGS) models. The main disadvantage of LES is the requirement of a very dense grid, especially in the near wall regions. Although the method cannot be applied for industrial systems (Spalart, 2000), it became very popular for simulations of lab-scale columns. Deen et al. (2001) compared Smagorinsky SGS model with $k − \varepsilon$ RANS model for E−E simulations of a square bubble column, using commercial software Ansys CFX−4.3. They investigated the key features of the highly dynamic flow with Bubble Induced Turbulence (BIT). The RANS model demonstrated an overestimation of the gas and liquid velocities, while LES simulations provided a good match with experimental data. Milelli et al. (2001) also reported poor accuracy of the $k − \varepsilon$ model, which fails in prediction of turbulence kinetic energy and dissipation rate in E−E simulations and leads to significant error in the calculated time-averaged liquid velocity.

Zhang et al. (2006) compared Smagorinsky and Vreman SGS models for the LES method using the E−E approach and experimental data of Deen (2001). Although the liquid and gas velocity matched for both models, the Smagorinsky model showed overestimation of the eddy viscosity in the near wall regions, while the Vreman model gave accurate results. In addition, the effect of the Smagorinsky constant in Vreman model was studied. A good agreement with experiments was found for the range $C_t = [0.08 \ldots 0.1]$, which is almost a factor two lower than the default value of the Smagorinsky constant ($C_t = 0.25$).

Hu and Celik (2008) also reported that for gas−liquid systems, modeled with the E−L approach, the Smagorinsky constant in the SGS model should be taken lower than for single-phase flows. (Bai et al., 2011) investigated Smagorinsky and Vreman SGS models using the DBM. Results were compared with experimental data from Deen (2001) and showed that the Vreman model is in better agreement with experimental data. The constant in both models was set to $C_t = 0.1$.

More fundamental results were reported by Labourasse et al. (2007) and Toutant et al. (2008), who proposed new subgrid closures for two-phase LES and reported good agreement with DNS simulation.

Ma et al. (2015, 2016) used Machine Learning to derive simple models for average bubble−liquid flow quantities. Authors used Model Averaging Neural Network and linear regression models. Trained systems showed good match with DNS results and demonstrate good performance. However, obtained models are not yet applicable to complex large-scale simulations.

To reduce high computational expenses of the LES in large-scale systems Spalart et al. (1997) proposed the Detached Eddy Simulation (DES) approach, which combines RANS and LES in one model. Masood and Delgado (2014) were the first to study a bubble column using DES in combination with the E−E approach. The authors employed Shear Stress Transport (SST) $k − \omega$ model in Ansys CFX-14.0 and reported quite good agreement with experimental measurements from Deen (2001).

The interest in the DES method is underpinned by its better accuracy and lower grid requirements in comparison with turbulence models based on RANS equations and the LES method, respectively. Thus, DES allows to obtain accurate resolution of turbulent structures in large-scale systems, where RANS and LES fail or are not applicable. In the present work the quality of different DES models (Spalart–Allmaras, $k − \varepsilon$ and $k − \omega$ SST), coupled with DSMC, is investigated for a gas−liquid flow with respect to experimental data reported by Deen (2001).

The paper is structured as follows. In Section 2 treatment of bubble dynamics is explained. Sections 3−5 provide explanation of the governing equations and used turbulence models. In Section 6 the main aspects of DES are described. Section 7 is dedicated to implementation details and numerical methods. Results are presented in Section 8 and finally conclusions are given in Section 9.

### 2. Bubble dynamics

For the present work, the developed and validated DSMC method of Kamath et al. (2017), is used to resolve bubble dynamics. In this method, the identification of the collision partner is treated in a stochastic manner, while collisions themselves are based on hard sphere collision rules. As in the original paper a two-way coupling of the gas−liquid system is employed.
The presence of the gas phase is accounted for by the voidage and momentum source terms in the governing equations for the liquid phase. Six forces are applied to each individual bubble: gravitational force, far-field pressure force, drag force, lift force, virtual mass and lubrication force. The wall, drag and lift forces coefficients are calculated according to Tomiyama (1998). To account for swarm effects, the drag closure proposed by Roghair et al. (2009) is employed.

The DSMC method imposes some restrictions on the size of the computational cells used for discretization of the governing equations: the bubble size should be less than the cell size.

3. Governing equations for the liquid phase

In the present work the system of full Navier–Stokes equations is used to describe the dynamics of the liquid phase. Momentum and continuity equations are given by

\[ \frac{\partial \rho_{li} u_{li}}{\partial t} + \frac{\partial \rho_{li} u_{li} u_{lj}}{\partial x_j} = -\alpha_i \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij} + \alpha_i \rho_{li} g_i + F_i \]  

(1)

\[ \frac{\partial \alpha_i}{\partial t} + \frac{\partial \alpha_i u_{li}}{\partial x_j} = 0 \]  

(2)

where \( \tau_{ij} \) is the local liquid volume fraction. The quantity \( F_i \) represents an external source term due to the presence of bubbles. The viscous tensor \( \tau_{ij} \) is given by

\[ \tau_{ij} = \mu_{eff} \left( S_{ij} - \frac{2}{3} \delta_{ij} \right) \]  

(3)

where the effective dynamic viscosity \( \mu_{eff} \) is calculated as a combination of molecular and eddy viscosities

\[ \mu_{eff} = \mu + \mu_t \]  

(4)

whereas the rate-of-strain tensor is given by

\[ S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(5)

Since we consider isothermal flow the molecular viscosity \( \mu \), as well as liquid density \( \rho_{li} \) and gas density \( \rho_g \) are constants in our simulations.

The system of Eqs. (1) and (2) remains unclosed until the eddy viscosity is determined. In the present work five different models are used to calculate this field. Among them we use two subgrid-scale models for LES method and three RANS models embedded into DES. These models will be described in the following sections.

4. SGS models

LES simulations are conducted with the Smagorinsky (SMG) and Vreman (VR) subgrid-scale (SGS) models. The SMG model was first proposed in 1963 (Smagorinsky, 1963) and is commonly accepted in different applications. However, the SMG may give non-zero values of the eddy viscosity at walls, since effects of solid surfaces on the subgrid viscosity are not taken into account. The problem can be overcome by modifying the initial model formulation or by using damping functions, which activate in the near wall regions (Piomelli et al., 1984). However, the primary interest of this work is the flow characteristics in the bulk of the domain. Although the grid refinement would eliminate the problem of the unresolved boundary layer, it cannot be used in the current study due to restrictions imposed by the DSMC method. Therefore, the model was utilized in its original formulation

\[ \mu_t = \rho (C_s \Delta)^2 S \]  

(6)

where \( C_s \) is a model constant taken equal to 0.1, \( \Delta \) is a cubic root of the grid cell volume and \( S \) is a modulus of the rate-of-strain tensor given by

\[ S = \sqrt{2 S_{ij} S_{ij}} \quad S = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(7)

An alternative to the SMG model is the VR (Vreman, 2004) SGS model, which has an improved treatment of the wall regions. The author also claimed other advantages, e.g. lack of explicit filtering and averaging and rotational invariance. The VR model has been proven to be accurate in simulations of highly dynamic gas–liquid flows (Zhang, 2007; Bai, 2010; Lau, 2013). The eddy viscosity is calculated with

\[ \mu_\epsilon = 2.5 \rho C_s^2 \sqrt{B_\beta} \]  

(8)

where

\[ \alpha_{ij} = \frac{\partial u_i}{\partial x_j}, \quad \beta_{ij} = \Delta_m \alpha_{mi} \alpha_{mj} \]  

(9)

\[ B_\beta = \beta_{11} \beta_{22} - \beta_{12}^2 + \beta_{11} \beta_{33} - \beta_{13}^2 + \beta_{22} \beta_{33} - \beta_{23}^2 \]  

(10)

Here \( \Delta_m \) is the cell size in \( m \)th direction (Vreman, 2004).

5. RANS models

5.1. Spalart–Allmaras model

The Spalart–Allmaras (SA) model is one of the most simplest RANS models available today. The model became very popular within the last decades because of its accuracy in many CFD applications. The SA model consists of only one transport equation written for the field of modified eddy viscosity \( \tilde{\nu} \), resulting in low computational expenses and relatively simple implementation.

The authors claimed that the model can be applied to both compressible and incompressible flows without any modifications. In the conservative form Allmaras et al. (2012) the SA model is given by

\[ \frac{\partial \alpha_i \tilde{\nu}}{\partial t} + \frac{\partial \alpha_i \rho u_i \tilde{\nu}}{\partial x_j} = \alpha_i \rho S_{\text{SA}} - \alpha_i D_{\text{SA}} + \frac{1}{\sigma} \frac{\partial}{\partial x_j} \left( \alpha_i \rho (\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right) + c_{\epsilon 2} \alpha_i \rho \frac{1}{\sigma} \left( \frac{\partial \tilde{\nu}}{\partial x_j} \frac{\partial \tilde{\nu}}{\partial x_j} - (\nu + \tilde{\nu}) \frac{1}{\sigma} \frac{\partial \tilde{\nu}}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} \right) \]  

(11)

where production and destruction terms are defined by

\[ P_{\text{SA}} = \rho c_{\epsilon 1} \tilde{\nu} \]  

(12)

\[ D_{\text{SA}} = \rho \left( c_{\epsilon 1} f_{\nu} - \frac{c_{\epsilon 1}}{K^2} \right) \left( \frac{\tilde{\nu}}{d} \right)^2 \]  

(13)

Here \( d \) represents the distance to the nearest wall. The modified eddy viscosity is proportional to the dynamic eddy viscosity as

\[ \mu_\epsilon = \rho f_{\nu} \]  

(14)

where

\[ f_{\nu} = \frac{X^3}{X^3 + C_{\epsilon 1}^2}, \quad X = \frac{\tilde{\nu}}{\nu} \]  

(15)

Additional terms in the Eq. (11) are given by

\[ \tilde{S} = \Omega + \frac{\tilde{\nu}}{K^2} f_{\epsilon 2}, \quad f_{\epsilon 2} = 1 - \frac{X}{1 + X f_{\nu}} \]  

(16)
\[ f_w = \frac{g}{\bar{S}} \left[ \frac{1 + c_2}{g^2 + c_2} \right]^{1/6}, \quad g = r + c_{w2}(r^2 - r) \] (17)

\[ r = \min \left[ \frac{\bar{S}}{\Omega_{1/2}}, 10 \right] \] (18)

\[ \Omega = \sqrt{2}W_i W_j, \quad W_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \] (19)

The term \( \bar{S} \) is limited according to the recommendations given in Allmaras et al. (2012)

\[ \bar{S} = \frac{\bar{S}}{k^2} f_{w2} \] (20)

\[ \bar{S} = \begin{cases} \Omega + \bar{S}, & \text{if } \bar{S} \geq -c_2 \Omega \\ \Omega + \frac{c_3}{(c_3 - 2c_2)}\Omega - \bar{S} & \text{otherwise} \end{cases} \] (21)

Note, that \( \bar{S} \) may become equal to zero, and therefore, to prevent problems in the evaluation of Eq. (18), the term \( r \) is explicitly set to 10. Model constants are taken unchanged from the original paper (Spalart and Allmaras, 1992), see Table 2.

At the walls the modified eddy viscosity is set to zero. At the outflow and pressure prescribed boundaries, the Neumann condition is imposed.

To improve the stability of the model, the production term \( P \) is treated explicitly, while the destruction term \( D \) is used implicitly in the following form

\[ D^{\text{new}} = \left( c_{w1} f_w - \frac{c_{w1}}{k^2} f_2 \right) \frac{\rho \bar{S}}{\partial t} \bar{v}_{\text{new}} \] (22)

where subscripts “new” and “old” refer to data from new and old time steps, respectively.

5.2. \( k - \epsilon \) model

The \( k - \epsilon \) (KE) model is one of the most popular turbulence models in engineering practice because of its robustness and accuracy. This model consists of two transport equations written for the turbulence kinetic energy \( k \) and its dissipation rate \( \epsilon \). In the present study the version of the model proposed by Lam and Bremhorst (1981) is used

\[ \frac{\partial \rho \bar{k} / \partial t} = \frac{\partial \rho \alpha_{1} k / \partial x_j} = \alpha_{l} p_{k}^{\text{KE}} - \alpha_{l} D_{k}^{\text{KE}} + \frac{\partial}{\partial x_j} \left[ \alpha_{i} \left( \mu + \frac{\mu_{l}}{\sigma_{k}} \right) \frac{\partial k}{\partial x_j} \right] \] (23)

\[ \frac{\partial \rho \epsilon / \partial t} = \frac{\partial \rho \alpha_{1} \epsilon / \partial x_j} = \alpha_{l} p_{\epsilon}^{\text{KE}} - \alpha_{l} D_{\epsilon}^{\text{KE}} + \frac{\partial}{\partial x_j} \left[ \alpha_{i} \left( \mu + \frac{\mu_{l}}{\sigma_{k}} \right) \frac{\partial \epsilon}{\partial x_j} \right] \] (24)

The production and destruction terms can be calculated with equations (25).

\[ p_{k}^{\text{KE}} = \tau_{ij} \frac{\partial u_i}{\partial x_j} \quad D_{k}^{\text{KE}} = \rho \epsilon \quad D_{\epsilon}^{\text{KE}} = C_{2} f_{2} \frac{\rho \epsilon^{2}}{k} \] (25)

Reynolds stresses and the rate-of-strain tensor are given by

\[ \tau_{ij} = \frac{1}{4} \left( 2 \sigma_{ij} - 3 \delta_{ij} \right) - \frac{2}{3} \frac{\rho \epsilon}{k^{2}} \delta_{ij} \] (26)

\[ S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \] (27)

The turbulent eddy viscosity is calculated from a combination of model constants and the \( k \) and \( \epsilon \) fields

\[ \mu_{l} = C_{1} f_{i} \frac{\rho k^{2}}{\epsilon} \] (28)

According to Lam and Bremhorst (1981), functions \( f_{i}, f_{1}, f_{2} \) and \( f_{\epsilon} \) are defined by

\[ f_{i} = [1 - \exp(-0.0165 Re_{r})]^{2} [1 + 20.5/Re_{r}] \] (29)

\[ f_{1} = 1 + (0.05/Re_{r})^{3} \quad f_{2} = 1 - \exp(-Re_{i}^{2}) \] (30)

where dimensionless parameters \( Re_{r} \) and \( Re_{r} \) are given by

\[ Re_{r} = \frac{\rho k^{2}}{\mu} \quad Re_{\epsilon} = \frac{\rho \sqrt{k d}}{\mu} \] (31)

Constants specified for the KE model are presented in Table 3.

At the walls kinetic energy of turbulence is set to zero, while the Neumann condition \((\partial k/\partial x_{w}) = 0 \) is applied to the dissipation rate, as recommended by Patel et al. (1985).

It is well-known that the robustness of the numerical implementation can be increased if negative terms are treated implicitly and positive terms are treated explicitly (Hirsch, 2007). Using the same procedure as for the SA model the destruction terms in Eqs. (23) and (24) can be re-written according to Eq. (32).

\[ D_{k}^{\text{new}} = \frac{\rho \epsilon / \partial t}{\partial x_j} \quad D_{\epsilon}^{\text{new}} = \frac{C_{2} f_{2} \rho \epsilon^{2}}{k} \] (32)

5.3. \( k - \omega \) SST model

The last RANS model considered in the present study is a Shear Stress Transport (SST) \( k - \omega \) model proposed by Menter (1994). The model represents a combination of more fundamental \( k - \epsilon \) and \( k - \omega \) models and gives an accurate resolution of the turbulent boundary layer, while the characteristics of the mean external flow are captured well. In the present study the SST-2003 (Menter et al., 2003) is implemented. The model is given by two equations for the
The production and destruction terms are given by

\[ P_{SST} = \tau_{ij} \frac{\partial u_i}{\partial x_j}, \quad D_{SST}^k = \beta^* \rho \omega k, \quad D_{SST}^\omega = \beta \rho \omega^2 \]  

(35)

The turbulent stress and rate-of-strain tensor are determined by Eqs. (36) and (37).

\[ \tau_{ij} = \mu_t \left( 2S_{ij} - \frac{2}{3}S \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij} \]  

(36)

\[ S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(37)

The expression for eddy viscosity is given by

\[ \mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, SF^2)}, \quad S = \sqrt{2S_{ij}S_{ij}} \]  

(38)

where \( S \) is a modulus of the rate-of-strain tensor. The function \( F_2 \) here is calculated by

\[ F_2 = \tanh \left( \left[ \max \left( 2 \frac{\sqrt{\frac{k}{\beta^* \omega d}} \frac{500 \nu}{d^2 \omega} \right) \right]^2 \right) \]  

(39)
Fig. 3. Comparison of experimental and simulated profiles of average axial liquid velocity at $H = 0.1575$ m (e–f), $H = 0.25$ m (c–d) and $H = 0.3375$ m (a–b). The results of LES with different SGS models are presented on the left, while the results of DES models are presented on the right.
The standard model constants used in the present study are listed in the Table 4.

At the walls, the turbulence kinetic energy $k$ is set to zero whereas the specific dissipation rate $\omega$ is calculated using the following expression

$$\omega_{\text{wall}} = 10 \frac{6\nu}{\beta_1 (\Delta d_1)^2}$$  \hspace{1cm} (45)$$

where $\Delta d_1$ is the distance between the wall and the center of the first cell. At the outlet or pressure prescribed boundaries, the Neumann boundary condition is imposed for both $k$ and $\omega$ fields.

For the sake of stability, the destruction terms in Eqs. (33) and (34) are treated implicitly, while production terms are taken explicitly. We found that the SST model may lead to divergence of the solution, if the $\omega$ field is not properly initialized. Therefore, in the present study, value $\omega_{\text{wall}}$ (see Eq. (45)) is used as an initial guess.

6. Detached Eddy Simulation

The main idea of the DES (Spalart et al., 1997) is employing a single turbulence model, which is acting as SGS model in regions where the grid resolution is fine enough to resolve turbulent structures, while in other regions the model is used as a pure RANS model. This combination allows for a less refined grid near the walls compared to LES, decreasing thereby the memory requirements and the computational costs. The DES procedure replaces the RANS length scale (Spalart et al., 1997), which is explicitly presented in most models, by a modified expression given by

$$L_{\text{DES}} = \min (L_{\text{RANS}}, C_{\text{DES}} \Delta)$$  \hspace{1cm} (46)$$

where $L_{\text{RANS}}$ is an original turbulence length scale of a RANS model, $\Delta$ is the LES filter limit, which is generally equal to the maximum grid cell size, and $C_{\text{DES}}$ is a constant analogous to the Smagorinsky one. The main advantage of the DES, compared to other hybrid RANS/LES approaches (Sagaut et al., 2006), is automatic transition between two branches of the model, as given by the Eq. (46).

The following subsections explain the main aspects with respect to the application of the DES procedure to RANS models, described in Section 5.

6.1. DES-SA

In a case of the SA model, the RANS length scale $L_{\text{RANS}}$ is determined by a distance to the nearest wall. Therefore, Spalart et al. (1997) suggested to replace $d$ in the original model with the modified distance to the nearest wall given by

$$d = \min (d, C_{\text{SA}} \Delta)$$  \hspace{1cm} (47)$$

Shur et al. (1999) performed simulations of the decay of homogeneous isotropic turbulence on the basis of the experimental data from Comte-Bellot and Corrsin (1971) and determined $C_{\text{SA}}$ as 0.65.

Replacing $d$ with modified $d$ in every equation of the SA model can easily lead to an unrealistic distribution of the eddy viscosity in the numerical domain (Breuer et al., 2003). A fast non-linear drop of the subgrid viscosity can be generated by the activation
Fig. 6. Comparison of experimental and simulated profiles of turbulence kinetic energy at $H = 0.1575$ m (e–f), $H = 0.25$ m (c–d) and $H = 0.3375$ m (a–b). The results of LES with different SGS models are presented on the left, while the results of DES models are presented on the right.
of the low-Re terms in the LES regions. To overcome this problem, Shur et al. (2003) proposed to use the new LES length scale

$$\hat{d} = \min \left( d_w, \psi \left( \frac{V_1}{V} \right) \frac{C_{SA \text{DES}}}{\Delta} \right)$$

where the limiting function $\psi$ is given by

$$\psi^2 = \min \left( 100, \frac{1 - \frac{C_{\text{SST}}}{{C_{\text{SA \text{DES}}}}}}{f_{f1}} \right)$$

Here, term $f_{f1}^{\text{DES}}$ denotes the model function $f_w$ calculated using $\hat{d}$.

6.2. DES-KE

The KE model consists of two equations and $L_{\text{RANS}}$ appears in different terms. The model length scale is given by

$$L_{\text{KE}}^{\text{RANS}} = \frac{k^{3/2}}{\epsilon}$$

and Eq. (46) is re-written to

$$L_{\text{DES}}^{\text{KE}} = \min \left( L_{\text{RANS}}^{\text{KE}}, C_{\text{KE \text{DES}}}^{\text{KE}} \Delta \right)$$

According to Strelets (2001) only the dissipative term in the equation of the turbulence kinetic energy (see Eq. (23)) should be modified as follows

$$D_{\text{DES}}^{\text{KE}} = \rho \frac{k^{3/2}}{L_{\text{DES}}^{\text{KE}}}$$

Strelets (2001) calibrated the model constant $C_{\text{KE \text{DES}}}$ and obtained very good agreement with experimental data for the value 0.61.

6.3. DES-SST

Similar to the KE model, the DES based on the SST replaces the RANS length scale only in the dissipative term of the equation of the turbulence kinetic energy (see Eq. (33)) as follows

$$D_{\text{DES}}^{\text{SST}} = \rho \frac{k^{3/2}}{L_{\text{DES}}^{\text{SST}}}$$

where $L_{\text{DES}}^{\text{SST}}$ is determined by

$$L_{\text{DES}}^{\text{SST}} = \min \left( L_{\text{RANS}}^{\text{SST}}, C_{\text{SST \text{DES}}}^{\text{SST}} \Delta \right)$$

Here, the $L_{\text{RANS}}$ is given by

$$L_{\text{RANS}}^{\text{SST}} = \frac{k^{1/2}}{\beta^{1/2}}$$

Since SST uses the blending function $F_1$ the constant $C_{\text{DES}}^{\text{SST}}$ should be calculated with Eq. (56)

$$C_{\text{DES}}^{\text{SST}} = (1 - F_1)C_{\text{DES}}^{\text{KE}} + F_1C_{\text{DES}}^{\text{SST}}$$

Strelets (2001) determined $C_{\text{DES}}^{\text{KE}} = 0.61$ and $C_{\text{DES}}^{\text{SST}} = 0.78$ by calibrating constants for both $k - \epsilon$ and $k - \omega$ DES models, separately.

7. Implementation details

All numerical simulations in the present study are performed using the new in-house code “FoxBerry”. Solutions are obtained in a full 3D formulation with implicit treatment of the convection and diffusion terms. Discretization is done using the Finite Volume method on an uniform Cartesian grid with staggered arrangement of the primary variables (Versteeg and Malalasekera, 2007). All convective fluxes are discretized using the second-order accurate stencil compact, a Deferred Correction (DC) method is used (Ferziger and Peric, 1999). The low-order scheme for the DC method is the first order upwind scheme. Time integration is done using a first-order backward Euler’s method. For the pressure–velocity coupling the SIMPLE algorithm (Patankar, 1980) is used.

All linear systems built after discretization are solved using BigStab(2) method (Sleijpen and van der Vorst, 1995). No preconditioners are used for momentum and scalar equations since only a few iterations are required for convergence. However, for pressure correction equation an Algebraic Multigrid method (Henson and Yang, 2002) is used as a preconditioner. All linear solvers are part of the in-house library and have been tested on several single- and multiphase problems.

Fig. 1 shows the geometry of the numerical domain used in the present study. No-slip boundary condition is imposed on all faces of the domain, except the top one, where free-slip boundary condition is used. Few cells at the top of the domain’s vertical sides, which are indicated by the black regions in Fig. 1, are set to pressure outlet to prevent mass conservation problems.

The sparger is modeled using 7 × 7 nozzles arranged in a square and is located exactly in the middle of the bottom wall. Bubbles are introduced into the domain simultaneously. Since no break-up or coalescence model is used, bubble sizes are preserved.

The gas and liquid physical parameters as well as numerical parameters used for the current study are presented in Table 5. Dimensionless parameters are calculated as follows

$$E_o = \frac{\rho g d_b^2 \rho_l}{\sigma}, \quad M_o = \frac{\rho l \mu_l \Delta \rho_0}{\rho_l^2 \sigma^3}, \quad Re_b = \frac{\rho_b d_b \rho_l}{\mu_l}$$

where $d_b$ is the bubble diameter, $\sigma$ is the maximum magnitude of the average relative bubble velocity, $\sigma$ is the surface tension, $\mu_l$ and $\rho_l$ are liquid dynamic viscosity and density, respectively. Three heights in the column (see gray lines, Fig. 1) are used to compare results of the present work with experimental data of Deen (2001) and numerical data from Masood and Delgado (2014). To obtain profiles of the average gas velocity, 30 averaging cubic volumes are created along lines of interest. At each time step, bubble velocities are volume-averaged for every cell as follows

$$\bar{v} = \frac{\sum_{i=0}^{N} v_i \Omega_i}{\sum_{i=0}^{N} \Omega_i}$$

where $\Omega$ is the volume of a bubble presented in the averaging cell, $v$ is bubble velocity and $N$ is the total amount of bubbles presented.
Fig. 8. Comparison of experimental and simulated profiles of average axial gas velocity at $H = 0.25$ m (e–f), $H = 0.2835$ m (c–d) and $H = 0.324$ m (a–b). The results of LES with different SGS models are presented on the left, while the results of DES models are presented on the right.
Fig. 9. Comparison of simulated profiles of average gas holdup at \( H = 0.25 \text{ m} \).

**Table 5**

Simulation parameters used for the bubbly flow simulations in a square bubble column (see Fig. 1).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column size ((D \times L \times H))</td>
<td>(0.15 \times 0.15 \times 0.45 \text{ m} )</td>
</tr>
<tr>
<td>Liquid density, ( \rho_l )</td>
<td>1000 ( \text{ m}^3 )</td>
</tr>
<tr>
<td>Liquid dynamic viscosity, ( \mu_l )</td>
<td>(1.002 \times 10^{-3} \text{ m} )</td>
</tr>
<tr>
<td>Gas density, ( \rho_g )</td>
<td>1 ( \text{ m} )</td>
</tr>
<tr>
<td>Gas dynamic viscosity, ( \mu_g )</td>
<td>(1.85 \times 10^{-4} \text{ m} )</td>
</tr>
<tr>
<td>Bubble diameter, ( d_b )</td>
<td>4 \text{ m}</td>
</tr>
<tr>
<td>Superficial gas velocity, ( v_s )</td>
<td>4.9 \text{ m}</td>
</tr>
<tr>
<td>Surface tension, ( \sigma )</td>
<td>(72.86 \times 10^{-3} \text{ m} )</td>
</tr>
<tr>
<td>Simulation time</td>
<td>200 \text{ m}</td>
</tr>
<tr>
<td>Time step</td>
<td>(10^{-4} \text{ m} )</td>
</tr>
<tr>
<td>Averaging time</td>
<td>10 ... 200 \text{ m}</td>
</tr>
<tr>
<td>Grid size</td>
<td>(30 \times 30 \times 90 )</td>
</tr>
<tr>
<td>Tolerance</td>
<td>(10^{-3} )</td>
</tr>
<tr>
<td>( E_0 )</td>
<td>2.15</td>
</tr>
<tr>
<td>(- \log(\text{Mo}) )</td>
<td>10.6</td>
</tr>
<tr>
<td>( Re )</td>
<td>800</td>
</tr>
</tbody>
</table>

in the cell at the time step under consideration. All-volume averaged velocities are averaged in time with number averaging. The width of the averaging volume, which plays a crucial role, is set to 6 \text{ cm} in order to obtain correct results.

### 8. Results and discussion

#### 8.1. RANS/LES regions

For convenience, in the next sections abbreviation DES will be omitted leaving only pure RANS model's name as an indicator of the type of simulation. First, dynamics of the DES branches are determined. Fig. 2 shows time-average fields of RANS (blue) and LES (dark red) modes at the vertical plane in the middle of the domain. It was assumed that during simulations RANS regions will be concentrated along walls of the domain and partially inside the bubble plume, where large scale vortical structures are not present and small-scale turbulence cannot be accurately resolved.

The SA model (Fig. 2(a)) shows the expected pattern, which is also in line with Eq. (48). Fig. 2(b) demonstrates that the SST model was extensively used in RANS mode in the region near the sparger. Also, a very thin layer of RANS branch can be seen along walls.

In contrast, the KE model shows very dynamic behavior of RANS and LES regions. The difference between all models can be explained by different expressions of RANS length scales, i.e. the SA model determines \( L_{\text{RANS}} \) as a simple function to the nearest wall, while the KE and SST models calculate \( L_{\text{RANS}} \) based on the local fields of the turbulent quantities (see Eq. (50) and (55)). In addition, \( C_{\text{DES}} \) is a fixed constant in the SA and KE models, leading to a fixed LES length scale during the entire simulation, while in the SST model \( C_{\text{DES}} \) is a function changing in the time.

The SA model tends to produce a laminar solution, when the system is initialized at rest and without presence of any bubbles in the domain. Therefore, the model is initialized from fields obtained with the Vreman model after simulating 2.5 s. Since flow disturbances were necessary only as an initial guess the modified eddy viscosity field \( \tilde{\nu} \) was approximated as 10% of the LES eddy viscosity field.

#### 8.2. Liquid velocity

Fig. 3 shows profiles of the average axial liquid velocity. As can be seen from Fig. 3(a), (c) and (e) the SMG model leads to underestimation of the liquid velocity along the middle line at all three heights. This might be resolved by a calibration of the model constant \( C_{\text{DES}} \). The VR model shows very good agreement with the experimental data at the middle height, \( H = 0.25 \text{ m} \), and overestimates axial liquid velocity in the region near the sparger, \( H = 0.1575 \text{ m} \). At the top, \( H = 0.3375 \text{ m} \), both the SMG and VR models give similar results. Concluding, the VR model is the most accurate model and therefore, will be used as a reference LES simulation.

Fig. 3(b), (d) and (f) show results obtained with DES models. The SA model significantly overestimates liquid velocity for all three heights at the center of the domain. Therefore, it is concluded that the bubble plume remains narrow and almost does not oscillate. The current implementation of the SA model is not applicable for simulations of highly dynamic gas–liquid systems, since the model demands a high grid density near the wall, which could not be satisfied in the current study due to DSMC restrictions as mentioned in Section 2.

Both the KE and SST models slightly overpredict axial liquid velocity along the middle line of the domain, at \( H = 0.1575 \text{ m} \) and \( H = 0.25 \text{ m} \), but produce better match with the experimental profile at \( H = 0.3375 \text{ m} \), in comparison with LES simulations.

The difference between numerical and experimental results at height \( H = 0.3375 \text{ m} \) is mainly related to the absence of the free surface in the present simulations, which leads to changes in pressure distribution at the top of the domain and fully ignores the dynamics of the free surface caused by the bubbles leaving the liquid phase.

The results of Masood and Delgado (2014) demonstrate significant deviation with the experimental points and current simulations in the near wall regions. However, the velocity profile from Masood and Delgado (2014) is closer to the experimental data at \( H = 0.3375 \text{ m} \), which is again related to different type of boundary condition imposed at the top of the domain in both studies. In addition, at all heights, profiles from Masood and Delgado (2014) are biased to the left. The reason of this offset is most probably related to the short period of time-averaging.

The deviation between results obtained with SST models from the present and reference simulations is caused by differences in implementation. In the present study the original blended constant \( C_{\text{DES}}^{\text{SST}} \) proposed in Strelets (2001), was employed, while in the work of Masood et al. \( C_{\text{DES}}^{\text{SST}} \) was fixed to the value of 0.99. Besides, the work of Masood and Delgado (2014) employs different discretization schemes and different approaches for description of phase–phase interaction.

Comparison of the average axial liquid velocity at height \( H = 0.25 \text{ m} \), obtained with the SST, KE and VR models, is shown in Fig. 4. Although the VR model is in better agreement with the
Fig. 10. Instant snapshots of the bubble plume for the tested turbulence models at times $t = 25$ s, 40 s and 55 s. From left to right the results for the SA, SST, KE and VR models are shown. Bubbles are colored with the magnitude of their velocities, where blue and red colors represent low and high values, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Experiment in the middle, it underestimates velocity magnitude on the right, where KE and SST provide a very good match with the experimental points. Moreover, the KE model leads to a more centered profile compared to other models.

Comparison of DES-based results with other LES-based simulations is shown in Fig. 5. As a reference data, results from Deen (2001); Darmana (2006) and Bai (2010) are used (see Table 1 for details). The results obtained with the VR model in the present study are in better agreement with the experimental data compared to reference simulations. Among all models, the KE and SST perform very well, showing good agreement with the experimental data. Slight difference between both models and experimental points may be caused by $c_{DES}$ constant, which should be considered as a numerical parameter, that has to be calibrated for each particular type of flow.

8.3. Turbulence kinetic energy

The profiles of the turbulence kinetic energy (TKE) are shown in Fig. 6. Both SGS models show slightly higher values than the experimental data. The turbulence is not fully damped in the near wall regions, which can be caused by the low grid resolution.

The SA model demonstrates significant overestimation of the TKE at the top level, showing intense turbulence generation, related to the proximity to the top wall. At the other two heights, TKE profiles are too narrow, indicating that the turbulence generation aside of the bubble plume is very low.
In contrast, the KE model shows good agreement with the experimental data in the region near the sparger. At the middle height the results for the KE model are slightly better compared to the SST model. At the top of the column both KE and SST models show similar results. At all three heights, the tested KE and SST models predict the magnitude of the TKE better in comparison with the results of Masood and Delgado (2014).

8.4. Dynamic eddy viscosity

Fig. 7 shows the distribution of the average dynamic eddy viscosity for five models tested in the present study. The SMG, SST and SA models show growth of the eddy viscosity in the near wall regions. In contrast, the KE model demonstrates adequate decrease of \( \mu_1 \) field. The resulting eddy viscosity obtained with the SA model is high in the middle of the domain, which causes an increase of the internal fluid friction and as a result the damping of fluctuations in the liquid velocity.

8.5. Gas velocity

Calculated profiles of the axial gas velocity are presented in Fig. 8. At all three heights the SMG model shows better agreement with the experiment than the VR model. However, both models overestimate the magnitude of the axial gas velocity. The same tendency was shown by different authors for E–L simulations, (Deen, 2001; Lau, 2013; Zhang, 2007; Bai, 2010). The results of Masood and Delgado (2014) demonstrate significant overestimation of the gas velocity, especially in the near wall regions. The SA model overpredicts the gas velocity at all three heights, while the SST and KE models are in better agreement with the experiment. The SST model shows a lower axial gas velocity in the region near the sparger and at the middle height compared to the KE model. Presented results demonstrate, that with the lack of proper boundary layer resolution, the KE and SST models capture the dynamics of the gas–liquid flow very well.

8.6. Gas holdup

The distribution of the time average gas holdup at \( H = 0.25 \) m is presented in Fig. 9. As can be seen the SST and KE models show similar results, demonstrating very symmetric profiles. The VR model shows very close to the KE and SST distribution, while the SMG model demonstrates lower gas fraction in the middle of the domain. Comparison is done with the results of Masood and Delgado (2014).

8.7. Plume dynamics

The dynamics of the bubble plume directly depends on how well turbulent structures are resolved. The SA model leads to significant reduction of the liquid velocity perturbations and the bubble plume oscillations compared to other models and experimental data, as seen in Fig. 10. Within this period of time, 25–55 s, the plume only slightly moves from one wall to another; see Fig. 10(a), remaining “compact” with very pronounceable core along the entire height of the domain. The SST and KE models show absolutely different behavior of gas inclusions compared to the SA model, see Fig. 10(b) and (c). Bubbles are more spread over the domain and are not only concentrated near the top of the column. The plumes are more dynamic, with significant changes in shape and size. In addition, the core of plumes is almost fully destroyed at the second half of the domain, which is not shown by VR model, see Fig. 10(d).

9. Conclusion

In the present work, the implementation of three RANS models (SA, KE and SST) for DES was investigated with respect to the capability to predict dynamics of a gas–liquid flow. Numerical results were compared with experimental measurements of Deen (2001), with LES simulations based on Smagorinsky and Vreman SGS models and with DES-SST results obtained with E–E approach by Masood and Delgado (2014). For the first time, DES was successfully applied in combination with an Euler-Lagrange formulation for the gas–liquid dynamics to the investigation of bubble column.

The simple and computationally inexpensive DES-SA model is not able to correctly predict mean liquid and gas velocities in the considered type of flow. This model significantly overestimates the average axial liquid and gas velocities. In addition, there is a lack of highly dynamic oscillations of the bubble plume. This behavior is caused by a wrong estimation of the turbulence kinetic energy aside of the bubble plume, which leads to damping of liquid velocity fluctuations.

Both DES-SST and DES-KE models show very good agreement with experimental data and LES simulations performed with Vreman SGS model. Profiles of average axial liquid velocity obtained with DES-SST model demonstrate better match with experimental points in comparison with results from Masood et al. The oscillations of the bubble plume and spreading of bubbles are well captured by both models. In addition, DES-KE and DES-SST models, produce a better agreement with experimental measurements in comparison with data from the reference LES simulations (Deen, 2001; Bai et al., 2011; Darmana, 2006).

However, it is important to mention that all DES models used in the present study utilized gas constants initially obtained for single-phase flows (Strelets, 2001; Spalart et al., 1997). It is well known, that these constants should be carefully calibrated for each particular code and discretization scheme. Therefore, in future work, it is of big interest to investigate the sensitivity of both DES-SST and DES-KE models to different \( C_{DES} \) constants.

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Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ijmultiphaseflow.2018.08.006.

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