Computational fluid dynamics comparison of two-equation turbulence models by studying hydrodynamic parameters in the distillation trays

Sadegh Abbasnia [1,*] Alireza Abbasnia [2]

[1] Iranian Research Organization for Science and Technology (IROST), Department of Chemical Technologies, Azadegan Highway, P.O. Box 33535111, Tehran, Iran

[2] Department of Chemical Engineering, University of Tabriz, Tabriz, Iran

Corresponding author E-mail address: Sadeghabbasnia1981@gmail.com

Abstract

A comparison was performed between three various (laminar, standard k-ε and standard k-ω) for the calculation of hydrodynamic parameters of a Nye tray. Air and water were selected as the gas and liquid phases. The liquid phase was only supposed as a complete turbulent phase and the standard k-ε the model was chosen for that in three simulations. On the other hand, the gas phase was simulated with the mentioned three models (laminar, standard k-ε and standard k-ω). The simulations were carried out in the froth regime and the framework of Eulerian–Eulerian. Entrainment and a couple of other hydrodynamic parameters were calculated for the industrial-scale Nye tray. Ultimately, the results illustrated that the selection of standard k-ω for the gas phase leads to more exact results for the hydrodynamic parameters. The obtained results from the standard k-ω model were close to experimental data than the two other models.

Key words

Standard k-ε model, standard k-ω model, laminar model, Nye tray, hydrodynamic parameters

1. Introduction

The two-equation turbulence Models have been the basis of a lot of turbulence model research over the past three decades. These models provide a calculation of k. as well, the mentioned models provide a turbulence length scale or equivalent. As a result, the models are two complete equations, meaning that the two-equation models can be utilized to predict the properties of a certain turbulent flow without prior knowledge. The standard k-ε turbulence model is the most practical model utilized in computational fluid dynamics (CFD) for simulating the medium flow characteristics for turbulent flow circumstances. This is a two-equation model that provides an overall description of turbulence utilizing two transfer equations. The primary motivation for the k- ε model was to progress the mixing length model, also to find another to determine turbulent length scales of medium to high complexity. (k) is the turbulence kinetic energy and (ε) is dissipation. In CFD, we need to estimate the Reynolds-averaged Navier-Stokes equations (RANS equations) by an appropriate equation and, the standard k–ω turbulence model is utilized for the sake. In this model, two partial differential equations for two variables (k) and (ω) are defined. (k) is the turbulence kinetic energy and, (ω) is the specific rate of dissipation [1].

Simulations of trays via CFD, have been performed over the past years frequently. Plenty of these simulations have been supposed to respectively two laminar and turbulent models for gas and liquid phase. Some of the studies have been done with two turbulent models for both phases. For example Gesit et al. [2] studied the hydrodynamic parameters of an industrial-scale sieve tray by computational fluid dynamics. They assumed the laminar model for the gas phase and the standard k-ε turbulence model for the liquid phase and the results were compared with experimental data. Rahimi et al. [3] investigated the weep rate of a rectangular sieve tray by CFD. The selected system was air –water and a k- ε model was used for both phases. The results were validated with experience correlations. Rahimi et al. [4] had a comprehensive investigation of the weep rate in an industrial- scale circular sieve tray via computational fluid dynamics and experiment. An Air-water system was utilized for the simulation and the k- ε model was selected for both phases. Plus the weep rate and pressure drops were studied too. All the results were compared with experimental data. A complete CFD comparison was performed between a few turbulence models in a structured packing by Ehsani et al. [5]. Dry pressure drop, irrigated pressure drop, mass transfer, and heat transfer were investigated via standard k- ε and k- ω models and the others for the gas phase and a k- ε model for the liquid phase. The results were validated by experimental data. Hosseini et al. [6] performed a study on a MellapakPlus 752. Y Structured Packing by CFD. They selected a couple of different turbulence models for the gas phase and compared the pressure drop in various models. Finally, the gained results were compared with conventional packing. A comparison of different turbulence models in predicting the temperature separation in a Ranque–Hilsch vortex tube was done by Dutta et al. [7]. Standard k–3, standard k– ω, and a few other models were used in the mentioned study and the results were validated with experimental data. Hosseini et al. [8] carried out an investigation on dry and wet pressure drops in a structured packing by CFD. A few turbulence models were used in the study and the results were compared with each other and experimental data. To describe the hydraulics and the flow pattern of a triangular fixed valve tray, a CFD model was developed by Sun et al. [9].they selected an air-water system and Eulerian framework for the simulation. The standard k- ε model was used and a couple of hydrodynamic parameters were investigated. Rahimi et al. [10] had research on hydraulic and mass transfer and efficiency of a rectangular sieve tray by computational fluid dynamics. They chose a methanol-n-propanol system in the Eulerian framework and, the standard k- ε model for the mentioned simulation. Finally, the effect of geometry on hydraulic and mass transfer and efficiency was investigated. Farsiani et al. [11] performed a study on the hydrodynamic characteristics of a valve tray via experiment and computational fluid dynamics. The air-water system and the standard k-ε model were used for the simulation. Several hydrodynamic characteristics were calculated by CFD and were compared with experimental data. A CFD investigation was done on the hydrodynamic behavior of conical cap trays via Zarei et al. [12]. The selected system was air-water and the VOF-like code framework was utilized. The Shear-stress-transport turbulence model was used for the simulation and pressure drops and the height of risers were studied. Malvin et al. [13] carried out a CFD study on flow regimes in a circular sieve tray using the droplet size distribution technique. A volume of fluid (VOF) framework and the standard k- ε model were used for the simulation of the complex flow phenomena in a tower. The analysis of droplet size distribution was used for characterizing the prevailing flow regime and the gained results were compared with experimental data. A complete experimental and CFD investigation on the hydrodynamic parameters of a ripple tray was carried out via Jiang et al [14]. The SST turbulence model was used and an Eulerian-Eulerian framework was selected for the CFD simulation. A few important hydrodynamic parameters were calculated by CFD and were validated via experiment. A numerical simulation of the gas-liquid flow behavior of the bubble cap tray was done by Kasiri et al. [15]. They developed a Computational Fluid Dynamic model to predict the hydrodynamic parameters of systems. A transient three-dimensional model in the Eulerian framework with a standard k-ε turbulence model was utilized in the mentioned study. Important hydrodynamic parameters were calculated and validated by experiments. Zhang et al. [16] had an investigation on gas flow field distribution of the tridimensional rotational flow sieve tray by computational fluid dynamics method. The realizable k- ε model was used for the simulations in the study and gas flow field distributions of TRST with different structural parameters, installation methods, and modified structures were investigated. Performance analysis and quantitative design of a flow-guiding sieve tray by computational fluid dynamics were done by Lei et al. [17]. They used a little experimental column to validate the results of the CFD model. For CFD modeling, the RNG k-ε model was utilized and the modified interphase momentum transfer term was incorporated into the simulation. The most important hydrodynamic parameters were investigated and the results were also compared with the sieve tray. Abbasnia et al. [18] studied on mass transfer of a conventional sieve tray and the same size Nye tray by CFD. The methanol- n-propanol mixing and the standard k-ε model and the Eulerian-Eulerian framework were used in the simulation. Murphree efficiencies were calculated for both trays and were compared with experimental data. A study on hydrodynamic parameters of an industrial-scale Nye tray by the experimental method was carried out by Abbasnia et al. [19, 20, 21, and 22]. They had a comprehensive investigation on parameters such as clear liquid height, froth height, pressure drops, weep rates, and entrainments in a Nye tray, and finally, the results were compared with the results of the same sieve tray. Current work deals with the comparison effects of 3 different models (2 turbulence models and 1 laminar model) in the results of CFD simulations for an industrial-scale Nye tray in the calculation of some of the hydrodynamic parameters and undesirable phenomena. The results of the simulation have been compared with experimental data. Regarding the introduction, the same studies have been done for a couple of other types of equipment such as packing but concerning fixed trays in towers, this subject rarely exists. On the other hand, a CFD study on entrainment in a Nye tray has not been carried out yet.

2. Simulation

2.1. Equations of the model

Continuity equations for both phases:

$$\frac{\partial(\varepsilon_L\rho_L)}{\partial t}+\nabla.(\varepsilon_L\rho_L u_L)=0 \tag{1}$$

$$\frac{\partial(\varepsilon_G\rho_G)}{\partial t}+\nabla.(\varepsilon_G\rho_G u_G)=0 \tag{2}$$

Momentum's equations:

$$\frac{\partial(\rho_L\varepsilon_L u_L)}{\partial t}+\nabla.\left(\rho_L\varepsilon_L u\,_L u_L-\mu_L\varepsilon_L(\nabla u_L+(\nabla u_L)^T)\right)=-\varepsilon_L\nabla p-M_{G,L}+\rho_L\varepsilon_L g \tag{3}$$

$$\frac{\partial(\rho_G \varepsilon_G u_G)}{\partial t} + \nabla.\left(\rho_G \varepsilon_G u_G u_G - \mu_G \varepsilon_G (\nabla u_G + (\nabla u_G)^T)\right) = -\varepsilon_G \nabla p + M_{G,L} + \rho_G \varepsilon_G g \tag{4}$$

$$\varepsilon_G + \varepsilon_L = 1. \tag{5}$$

Drag force, $\boldsymbol{M_{GL}}$:

$$M_{GL} = \frac{3}{4} \rho_L \frac{\varepsilon_G}{d_G} C_D (u_G - u_L)|u_G - u_L| \tag{6}$$

Drag coefficient, C_D:

$$C_D = \frac{4}{3} \frac{\rho_L - \rho_G}{\rho_L} g d_G \frac{1}{V_{Slip}{}^2} \tag{7}$$

Slip velocity, V_{slip}:

$$V_{slip} = \frac{U_G}{\varepsilon_G{}^B} \tag{8}$$

Average volume fractions, ε_G^B andε_L^B:

$$\varepsilon_L^B = exp\left[-12.55\left(U_G \sqrt{\frac{\rho_G}{\rho_L - \rho_G}}\right)^{0.91}\right] \tag{9}$$

$$\varepsilon_G^B = 1 - \varepsilon_L^B \tag{10}$$

Pressure fields, P:

$$P_1 = P_2 \tag{11}$$

The liquid phase was only supposed as a complete turbulent phase and the standard k- ε model was selected for that in three simulations. On the other hand, the gas phase was simulated with the three models (laminar, standard k- ε and standard k- ω). The simulations were done in the framework of Eulerian–Eulerian and the froth regime.

2.2. Boundary conditions

1-The inlet liquid velocity:

$$U_{L,in} = \frac{3Q_L}{2A_{in}}\left[1 - (\frac{z}{L_W})^2\right] \tag{12}$$

2-The inlet gas velocity:

$$F_S = U_G\sqrt{\rho_G} \tag{13}$$

$$U_{G,in} = \frac{U_G A_B}{A_H} \tag{14}$$

3- The same pressure of both phases at the outlet, assuming relative pressure at the outlet is zero.
4- No-slip condition for liquid and free slip for gas in the walls.

2.3. Geometry and meshing

Table1 shows the characteristics of the Nye tray in this study and figures 1 and 2 depict the geometry and meshing respectively.

3. Results

3.1. Dry pressure drop

Dry gas pressure drop versus F_S has been depicted in figure 3. the figure shows all three models (laminar, standard k-ε and standard k-ω) lead to close results for the dry pressure drop for the Nye tray when the F-factor is under around 0.05 (m/s (kg/m^3)$^{0.5}$). The phenomenon can be due to low gas velocity passing through the holes and lower turbulence of the gas phase than high F-factors. For F- factors more than 0.05, the differences between all three models are raised. Laminar and standard k-ε models have more errors rather than the standard k-ω model. The laminar and the standard k-ε models lead to lower and higher dry pressure drop amounts respectively.in comparison, the standard k-ω model results are closer to experimental data.

3.2. Total pressure drop

Figure 4 illustrates the total gas pressure drop versus various F-factors and the liquid flow rate (Q_L) is 0.0105 m^3/s.as can be observed, the changes are more intensive compared to the previous figure (figure 3).a low F_S in all three models (laminar, standard k-ε and standard k-ω) results in close total pressure data. After passing the F_S from about 0.05 (m/s $(kg/m^3)^{0.5}$), the variation of total pressure drops increases quickly. The standard k-ω model results have lower changes compared to the two other models. The changes for standard k-ε models are toward raising and concerning the laminar model, the changes go to reduction. It seems, the results of the standard k-ω model are more close to experimental data. Concerning the comparison between figure 3 and figure 4, (the dry pressure drop changes and the total pressure drop changes) it can be mentioned, the total pressure drop is more sensitive to raising F-factors than the dry pressure drop for all three models. It seems this phenomenon is because of the liquid phase's existence leading to different turbulence for the gas phase. Figure 5 depicts the gas velocity vector for the Nye tray in the dry state.

3.3. Entrainment

A comprehensive comparison of entrainment has been shown in figure 6. The liquid flow rate (Q_L) is 0.0105 m^3/s.it seems the trend of entrainment versus F_S, is the same two previous figures. For low F-factors, all three models (laminar, standard k-ε and standard k-ω) have almost the same results and are close to the experimental data. Enhancement of the F-factor results in a positive error for the results of the standard k-ε model and a negative error for the results of the laminar model and a positive error for the results of the standard k-ω model. In comparison, the standard k-ω model's errors are smaller than the standard k-ω model's errors.

Figure 7 shows the liquid velocity contour for the Nye tray at Q_L= 0.0105 and F_S = 1.015 (m/s $(kg/m^3)^{0.5}$).the figure shows the liquid velocity changes in the length of the Nye tray and doesn't have a big change in the width of the Nye tray.

3.4. Clear liquid height

Figure 8 shows the clear liquid height based on F-factors and in 0.0105 m^3/s liquid flow rate (Q_L).there are a couple of differences between the graph's trends of figure 8 and previous figures. It sounds like both turbulence models standard k-ε and standard k-ω have close results for the clear liquid height. It means to calculate this parameter, both of the two mentioned models are suitable and lead to almost the same negative errors with the experimental data. The laminar model has a higher error with the experimental data and it can be said the laminar model is not exact enough. On the other hand, this model results in positive errors against standard k-ε and standard k-ω models.

Figure 9 illustrates the liquid velocity vector on the Nye tray. Part (A) depicts the liquid vectors from the inlet downcomer to the outlet weir. Part (B) depicts a comparison between liquid vectors in the middle of the Nye tray (shape 1) and liquid vectors near the circumference of the Nye tray (shape 2). Liquid vectors' deflection is obvious in shape 2.

3.5. Froth height

Figure 10 illustrates the froth height based on F-factors and in 0.0105 m^3/s liquid flow rate (Q_L). The results of two models (standard k-ε and standard k-ω) are partly close to each other and the experimental data. It sounds like the laminar model causes a negative deflection of results from experimental data. Right like previous figures, for F-factors under about 0.05($m/s\ (kg/m^3)^{0.5}$), all three mentioned models lead to suitable results and the results have a suitable agreement with the experimental data, but when the F_S enhance, the errors of the models appear and the error of the laminar model is more than the two other models for high amounts of F_S.

4. Discussion and conclusion

This study aimed at a comparison via CFD between three models (laminar, standard k-ε and standard k-ω) for the calculation of hydrodynamic parameters for an industrial scale Nye tray. Air and water were chosen as the gas phase and liquid phase respectively. For the Liquid phase standard k-ω was selected in three simulations. The gas phase was simulated with three various turbulence models and the gained results were compared together and with experimental data. Overall it can be mentioned all three models have partly good results for the hydrodynamic parameters in low F-factors (around $F_S<0.05$). The laminar model doesn't have enough accuracy to calculate the hydrodynamic parameters of the tray when the F-factors are raising and the standard k-ε and the standard k-ω are more accurate than the laminar model and the standard k-ω leads to some better results than the standard k-ε in high amounts of F_S. The common regime for the two-phase mixture on the trays is the froth regime. It seems when the velocity of the gas phase is increased, the turbulence of the gas phase and the mixture of the two-phase get enhanced while the regime of the flow on the tray is still the froth regime, in this case, if the velocity of gas phase gets raised frequently, the flow regime on the tray approaches to spray regime in the near future. Finally, this subject results in big turbulence for the flow on the tray and all three models will not be able to guess the wanted results correctly. Generally, it appears the selection of turbulence models for the gas phase such as the standard k-ε or the standard k-ω is reasonable and essential, however, due to simplicity, plenty of studies have been performed with the gas phase laminar model, but it seems for flexible conditions and various flow rates complex models (such as the standard k-ε or the standard k-ω) are better. As well as, it appears the standard k-ω leads partly to more suitable results than the standard k-ε.

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