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Analysis of Two-Phase Pressure Drop in Structured Packings by Computational Fluid Dynamics

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ABSTRACT

Packed towers are continuous contact systems in which unlike tray towers, the liquid phase is dispersed, and the gas phase is continuous. Packed or packed distillation towers are widely used in chemical industries. The use of such towers is preferable to tray towers, especially in vacuum distillation operations. These columns are suitable in low pressure-drop or low liquid hold up operations. In this study, the pressure drop for the air-water system was simulated, and presented by a 3D model consisting of two layers of Gempak 2A structured packings by using computational fluid dynamics. Computational Fluid Dynamics is a useful tool for scale-up, design and optimization of chemical engineering equipment for its detailed prediction of hydrodynamic characteristics. The BSL turbulence model was used for simulation. The total number of meshes were 1315200. The simulation results were compared with laboratory and existing experimental data. The simulation error of the two-phase pressure drop compared with experimental data was 16.6%. The results of prediction agree well with the experimental data indicating the suitability of the proposed method for the simulation of the hydrodynamics in structured packed columns. The results of this study can be used in the hydraulic design of packed towers containing structured packings.

1. Introduction

Structured packings offer high mass transfer efficiencies compared to irregular packings and trays, and are widely used in many chemical industries, especially in distillation and extraction units. [1]. In 2001, Loser et al. [2] conducted a CFD analysis of gas distribution in Mellapak 250Y structured packings and reported single-phase pressure drop-in structured packing. The geometric model proposed in that research was very simple and consisted of only one channel of an element. The simulation results were compared only with theoretical models, and the average error was 15%. In 2006, Haghshenas Fard et al. [3] used CFX software to examine the characteristics of packed towers containing structured packings. They determined the mass transfer and the separation efficiency in the distillation process. Due

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to the complexity of the model, and its governing equations, a three-dimensional model consisting of two structured packing plates was proposed. The hydrodynamic parameters of packed towers, including single-phase and two-phase pressure drop and gas-phase distribution in the bed, were also investigated. In 2009, Jiangbo [4] used CFD analysis in a three-dimensional model consisting of two intersecting channels to study mass transfer and liquid hold-up at different pressures, and compared the results with laboratory data. Fluent software was used for modeling. In 2017, Mazarei Sotoodeh et al. [5] at the University of Sistan and Baluchistan investigated effect of geometry on hydrodynamics and flow description in MCSP modules with the help of the VOF model. The results showed that the average relative errors for dry and wet pressure drop prediction were 17% and 7% for MCSP-11 and 11% and 12% for MCSP-12, respectively. In 2020, Zivdar and Shah Mohammadi [6] reported the two-phase pressure drop in Sulzer BX structured packings by computational fluid dynamics and compared it with laboratory data. The percentage of relative error was reported to be 9.1%. Comparing the results of pressure drop in perforated plates with the results of pressure drop in simple and non-perforated plates, the pressure drop in perforated plates was decreased by 7%. In 2020, Hassanvand et al. [7] reported pressure drop and mass transfer efficiency of PACK-1300Y with a specific surface area of 1300 $\frac{m^2}{m^3}$, using computational fluid dynamics. The main approach of this research was to evaluate the main features of PACK-1300Y, including dry and wet pressure drop and HETP. To evaluate the HETP, and dry/wet pressure drop, the dynamic modeling of the computational domain was three-dimensional according to the Eulerian-Eulerian multiphase approach. In 2021, Tan et al. [8] explored a Eulerian-Eulerian three-dimensional computational fluid dynamics simulation approach. Air-water was used to simulate two-phase flow. The simulation results showed that the pressure drop increases with increasing gas or liquid flow rate. Liquid flow significantly affects the pressure drop, and liquid hold up. In 2021, Shahmohammadi et al. [9] analyzed dry pressure drop in structured packings using computational fluid dynamics. The packing was Sulzer-BX with 500 $\frac{m^2}{m^3}$ specific surface area. Simulation results were in good agreement with experimental data. The present study aims to simulate two phase pressure drop in an industrial tower packed with structured packages by CFD, and compare the results with experimental data.

2. Pressure drop model

Pressure drop and effective area are important parameters in the performance of packed towers. In the simulation performed in this research, only the equations of continuity and momentum were used. The multiphase system consisted of a mixture of two-phase, in which each phase has a different flow field. The equations used in this simulation were mass and momentum balances, which are as follows [10]. The equations of mass and momentum balance in the software were used in this research. The method of elliptic partial differential equations was used to generate the meshes.

$$\frac{\partial}{\partial t}(\rho) + \nabla.(\rho v) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho v) + \nabla.(\rho vv) = -\nabla.P + \nabla\left[\mu(\nabla v + v^T)\right] + \rho g + F \tag{2}$$

3. Simulation steps

There has been emergence of computational fluid dynamics in the academic and industrial use to model two-phase flows using volume of fluid technique. Volume of fluid technique is a special case of Eulerian-Eulerian multiphase

flow model that simulates two fluids separated by distinct resolvable interfaces. The numerical solutions of unsteady state Reynolds averaged continuity and Navier Stokes equations are provided by CFD simulations. The governing equations based on the homogeneous multiphase flow model have been solved using the CFX 11.

To model a system by using CFD, the general steps must be performed in order: first, the production of model geometry by Gambit software, then determining the boundary conditions of the model and meshing, then transferring the meshed geometry to CFX software. The modeling and formulation comprise the selection of basic equations governing the model, the initial conditions for the simulation, and the criteria for the evaluation of results.

The computational time required for each simulation run was about 6–7 days on a Pentium 4, CPU running on four 3.2 GHz cores with 4 GB of RAM. The BSL model (baseline k-ω model), which was a combination of the k-ω model near the surface and the k-ε model in the outer region, was used for the simulations.

3.1. Production of model geometry

To simulate structured packings by computational fluid dynamics various researches have been done so far and various geometrical models have been proposed. The closer the computational model was to the actual state of structured packings, the more accurate the results. The structured packing geometry is shown in Fig. 1. The geometric characteristics of the simulated structured packing are presented in Table 1. Experimental data have been obtained in a tower with an inner diameter of 0.43 m, and a bed height of 3.25 m at atmospheric pressure [11].

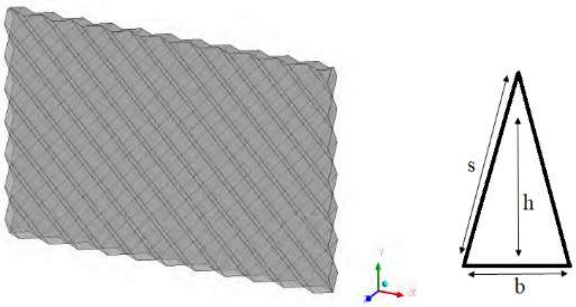


Fig. 1. The geometry of structured packing

Table 1. Geometric characteristics of structured packing

Type of structured packing	Surface Area (m^2/m^3)	Porosity (%)	Structured Angle	Dimensions of the triangular channel (m)		
Gempak 2A	223	95	45	b	s	h
				0.0267	0.018	0.0122

3.2. Mesh independence

To choose the right size for the mesh, answers must be obtained that are independent of the mesh size. This means that by changing the size of the mesh, no change in the response is observed. The meshed model with regular mesh structure with the number of meshes 1315200, 771584, and 1657700 was evaluated, and it was found that the simulation results with the number of meshes 1315200, and 1657700 were almost the same. Therefore, 1315200 meshes were selected as the appropriate number of meshes for the model. The geometry of the meshed structured packing is shown in Fig. 2. The meshes are hexagonal. Gambit software has been used for meshing.

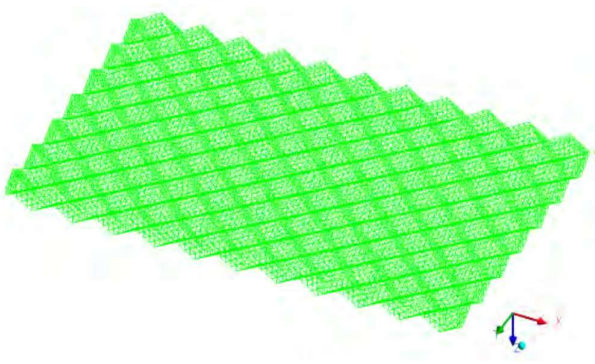


Fig. 2. Meshed geometry

3.3. Boundary conditions

Gas-liquid two-phase flow in the counter-current flow model was used in this system. The gas-phase was the air with a density of 1.185 kg/m^3, and the liquid phase was water with a density of 998 kg/m^3. The lower level of the packed bed was considered the input of the gas phase, and the upper level of the packed bed was considered the output of the gas phase. By having the volumetric fraction of one phase, the volumetric fraction of the other phase can be obtained by reducing that volumetric fraction from one. For both phases, the output boundary condition was considered "output pressure". For the walls, the boundary condition of the solid wall was assumed, i.e., assuming zero velocity for the fluid.

4. Results and discussion

Fig. 3 shows the pressure contours for the two-phase flow on a plate in the packing center. The apparent velocities of the gas and liquid phases, in this case, are 2.03 and 0.007 m/s, respectively. The reduction of pressure from the bottom to the top of the bed can be clearly seen. In this Figure, there are points along the bed with increasing and decreasing pressure, periodically. In these areas, which are actually intersecting channels, the incoming flows collide and the pressure increases.

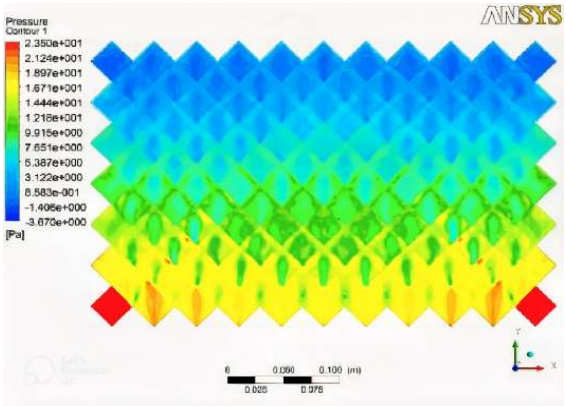


Fig. 3. Pressure contour for two-phase flow

Fig. 4 shows the liquid velocity contours. From this Figure, it can be shown that the liquid has a uniform distribution over the packing surface. At constant liquid flow rate, with the increase in the gas flow rate, the pressure drop also increased, which is a confirmation of the correctness of hydrodynamics.

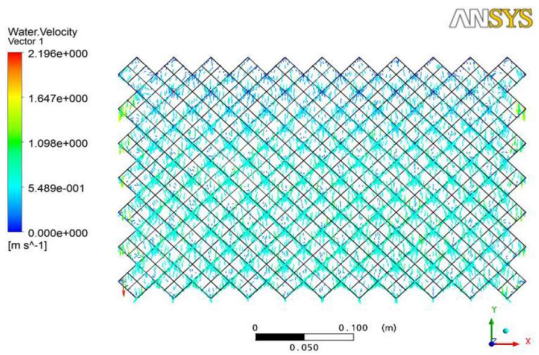


Fig. 4. Liquid velocity contours

Fig. 5 shows simulated two-phase pressure drop compared to the experimental results. The experimental two-phase pressure drop is given in Table 2. The apparent velocity of the liquid phase is 0.007 m/s. F factor is defined as superficial gas velocity multiplied by square root of gas density. The pressure drop has increased with the increase of the F factor. In this Figure, the simulation results are in good agreement with the experimental data. Therefore, this model can be used to investigate other parameters in structured packings. Simulations have been performed for water velocity of 0.007 m/s and different gas capacity factors ($Fs = u_G \rho_G^{1/2}$).

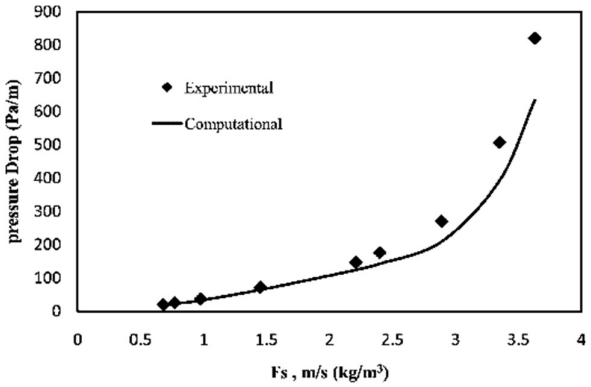


Fig. 5. Comparison of the simulated and experimental two-phase pressure drop

At higher gas flow rates, due to the higher liquid hold up, and also the error caused by the turbulence model, simulation error has increased.

Table 2. Experimental two-phase pressure drop

$F_s \frac{m}{s} (\frac{K_g}{m^3})^{0.5}$	$(\frac{P_a}{m})_{exp}$
0.681	19.4
0.77	25.5
0.977	36.9
1.45	71.6
2.21	147
2.4	176
2.89	270
3.35	507
3.63	820

5. Conclusion

In this research, two-phase pressure drop in the tower containing structured packings were discussed and investigated. For this purpose, at first, a geometric model of Gempak 2A structured packing was generated by Gambit software, and after meshing, it was evaluated by CFX-11 software. In order to confirm the results obtained from CFD simulation, a comparison was made between these results with experimental data. At fixed liquid rate, with increase of the gas velocity, the two-phase pressure drop increases. The lowest pressure drop obtained was related to the air velocity of 0.63 m/s and equals to 38.17 Pa/m. The highest-pressure drop was at the gas velocity of 3.34 m/s and equals to 285.34 Pa/m. The average relative error calculated from the simulation compared to the experimental data is 16.6% for the two-phase pressure drop.

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