Prediction of cross flow mixing in the structured packed bed through CFD simulation using (FBM and PMM) and validation with experiments

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ABSTRACT
This study focuses on prediction of cross flow mixing in structured bed by using O$_2$ molar concentration through CFD simulation. The mixing of the axial flow with cross flow in structured bed have been studied experimentally in a test box. The test box containing a 924 spherical particles of 52 mm diameter were arranged to achieve the simple cubic configuration which leads to a porosity of 0.48. Three-dimensional computational fluid dynamics (CFD) simulations have been carried out corresponding to the experimental setup. ANSYS 14 was used for CFD simulation with standard k-\( \varepsilon \) turbulence model. Fixed bed model (FBM) and porous media model (PMM) are used in this numerical work. Three different methods of contact point treatment are considered to obtain results using FBM. Moreover, results obtained through FBM (gap method) and PMM were also compared. Cross flow mixing takes place between N$_2$ entering via side injection and air entering at the bottom of the test box. Parametric variables are; lance diameter, lance position, and volume flow rate ratio. It is shown that results of CFD simulations using FBM can predict the cross flow mixing reasonably. The curves for O$_2$ concentration obtained through PMM are shifted little bit away from curves of FBM. It is also interesting to note that results of FBM with gap method fit best with the experimentally data.

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CFD; cross flow mixing; packed bed; simple cubic; contact point; and porous medium

Highlights
• CFD simulation and experiments were conducted for a simple cube packed bed.
• Mixing flows were simulated using the standard k-\( \varepsilon \) turbulence model at fixed bed model (FBM) and porous media model (PMM).
• Results obtained from the gap method are fitted best with the experimental data.
• The lance penetration depth has an influence on the O$_2$ concentration in the bed.
• O$_2$ concentration curve for PMM are shifting from that for FBM with a porosity of 0.48.

1. Introduction
Packed beds are widely applied in diverse areas of industry, such as shaft kilns, heat storage systems, cooling/heating of granular materials, chemical process industries and distillation processes. Therefore, it is of great importance to understand the details of flow information in the packed bed for practical applications. A shaft kiln is basically a packed bed reactor and works on a simple principle. The raw material is fed at the top of the kiln and the product is withdrawn from the bottom. For the thermal treatment of the material fuels are injected in the shaft through the wall using nozzles in the circumferential direction. From the bottom comes air which has to cool the material. This air mixes with the radially injected fuel and a part of radially injected additional combustion air (Unaspekov & Strekalova, 2002). A good mixing is important for the temperature homogenization in the cross section and therewith for the quality of the product. However, there is less knowledge about the mixing mechanism in packed beds. Therefore, the impact of measures to influence the mixing is not known, because of the geometric complexity, the movement of the lumpy processed materials and the height temperatures (about 1300°C). The measuring of main parameters, such as temperature, species, and velocity, is impossible. As a consequence, the CFD simulation is used to research the mixing. However, only a small section of a packed bed can be simulated because of the required small grids between the particles. Therefore, this study is focused on the mechanism of meshing the gas volume and particle contact and the influence of some parameters. The investigations of packed beds in the literature focus on flow,
heat and mass transfer, and pressure drop. Due to computer speed limitations, earlier works have been done on a small part of fixed packed bed to represent the flow between the particles. These works used a part of packing or a unit cell with periodic boundary conditions. In the last years, and with the progress in computational capability, it became of interest to represent a packed bed by a realistic approach with acceptable time and cost constraints. Almost all simulations of full beds were conducted with spherical packing to avoid the difficulties of generating a realistic packing of an arbitrary shape of particles such as point of contact. The CFD simulation results in confidence validated by obtained and verification Augier, Idoux, and Delenne (2010), Theodoros and Eugeny (2009), Guardo, Coussirat, Recasens, Larrayoz, and Escaler (2006) and Kuroki, Ookawara, Street, and Ogawa (2007) used the particle Nusslet number correlations to validate the simulation results for heat transfer between solid and fluid in a packed bed. Theodoros and Eugeny (2009), Augier et al. (2010), Reddy and Joshi (2008), Magnico (2003) and Ookawara, Kuroki, Street, and Ogawa (2007) have computed the pressure drop and compared it with correlations available in literature for packed bed. This study investigates the CFD simulation concerning contact point treatment for cross flow mixing in a packed bed. The CFD results are validated with the experimental data from a test rig.

There are two principal categories of packing: randomly packed bed and structured packed bed. The randomly packed beds are predominate in the industry because of their easy use and low price compared to other packing methods, moreover in scientific work structured beds are used because of small domains. Even for small domains the number of particles is strictly limited. Dixon, Walls, Stanness, Nijemeisland, and Stitt (2012), Ahmadi Motlagh and Hashemabadi (2008), Dixon and Nijemeisland (2001) and Calis, Nijenhuis, Paikert, Dautzenberg, and Bleek (2001) have performed simulations for full structured packed beds at low aspect ratio (tube to particle diameter ratio) for less than 50 particles. Other studies (Bai, Theuerkauf, Gillis, & Witt, 2009; Eppinger, Seidler, & Kraume, 2011; Baker & Tabor, 2010) simulated unstructured beds with particles ranged between 100 to 1000 particles. In order to create a geometric model of this bed including a large number of particles there are some limitations for instant such as the large number of cell elements required for mesh generation. Dixon et al. (2012) validated the CFD simulations of the heat transfer in fixed beds of spheres by comparing the results with experimental measurements in a pilot-scale rig. They used three methods: gaps, bridges, and flattening at contact points. The results revealed that the gap method gave poorer results compared to the other two bridge methods. Augier et al. (2010) used the CFD simulations to investigate the transport and transfer properties inside packed beds of spherical particles. They computed the heat and mass transfer properties in the packing. They solved the contact point’s problem between particles by applying a contraction of 2% of all particles of the bed. Yang, Wang, Zeng, and Nakayama (2010) studied numerically the flow and heat transfer inside small pores of novel structured packed beds. Wen and Ding (2006) experimentally measured the axial and radial distribution of temperature through a packed bed under the constant wall temperature. One of the studies for mixing in a bed with rectangular cross-section for non-reacting jet injection was investigated by Liscinsky and True (1992); the study revealed the mixing improves continuously with increasing momentum flux ratio, the mixing is more dependent on injector geometry than a mass flux ratio. Nirmolo, Woche, and Specht (2008) studied numerically the temperature homogenization of reactive and non-reactive cross flow. A cylindrical chamber with multiple jets injected radially was used. The maximum temperature difference over the chamber cross-sectional area was defined as a parameter to check the mixing quality. They showed that the mixing depends on the ratio of the two momentum flows divided by the square of the number of nozzles. Xu, Woche, and Specht (2009) proved that the momentum flux ratio was not a dominant factor on the jet penetration in packed beds because the flow hit the packing material immediately after being injected into the bed. Nirmolo et al. (2008) and Xu et al. (2009) showed that the momentum flux ratio in the most important parameter. Xu et al. (2009) used 100 mm spheres with a gap of 6 mm. An influence of momentum flux ratio was not seen. They developed a 3D geometry using the porous media model for three different porosity 0.4, 0.6, and 0.8, respectively. The results compared with discrete particle geometry. By application of the porous media model, the penetration of the combustion gas was under predicted for a porosity of 0.4, to achieve a deeper penetration, porosity must be bigger.

Bu, Yang, Dong, and Wang (2014, 2015a, 2015b) made a series of experimental studies by using the electrochemical techniques. They investigated the transition flow in the packed beds of spheres with different particle sizes experimentally. Wu and Ferg (2010) and Nijemeisland and Dixon (2004) used two main methods in CFD approach to create the geometry for a closely packed bed: the porous medium approach and the realistic discrete particle approach. In a porous media approach, the geometry of a packed bed is represented as an effective porous medium. This approach is used for a wide variety of single phase and multiphase problems, including flow through packed beds, filter papers, perforated plates, flow
distributors, and tube banks (Guo, Ying, Ni, & Abdou, 2006; Rooyen, Krueger, Matheos, & Kleingeld, 2006).

All these studies showed that there is much knowledge of flow transition, mass transfer, and pressure drop in randomly and structured packed beds. Based on these previous studies, there is much knowledge of flow transition, mass transfer, and pressure drop in randomly and structured packed beds. However, the mixing behavior of an axial flow with a radially injected flow has yet not been investigated.

2. Experimental setup

The experimental setup is shown in Figure 1(a). The operating conditions are represented in Table 1. The test section box has a length of \(L = 0.624\) m, a width of \(B = 0.364\) m and a height of \(H = 0.6\) m. The packed bed consists of ceramic spheres with 52 mm diameter. Ambient inlet air was blown to the packed bed through a perforated plate with an open area of 9% (high flow resistance) located at the bottom of the test section. This perforated plate ensured a good distribution of the air. The air volume flow rate was measured using rotameter with an error of \(\pm 0.015\) m\(^3\).s\(^{-1}\). Different axial air flow rates \((V_{\text{ax}} = 40, 83, 150, \text{ and } 250 \text{ m}^3 \cdot \text{h}^{-1})\) were tested. Nitrogen was injected perpendicularly to the air flow through a side lance attached to the box wall as shown in Figure 1(a). The nitrogen flow (injection flow) is supplied from a package of N\(_2\) bottles. Injected nitrogen is measured by rotameter with an error of \(\pm 0.01\) m\(^3\).s\(^{-1}\). Three injection flow rate boundary conditions \((\dot{V}_i = 5, 15 \text{ and } 25 \text{ m}^3 \cdot \text{h}^{-1})\) were tested with different inner diameters of 6, 12, and 20 mm. The experiments were done with lance injection depths of 0, 0.156, and 0.312 m. The packing arrangement was Simple Cubic (SC) as shown in Figure 1(a). In the present study, packing arrangement is identified by three parameters, namely: layers, columns, and rows. Layers are the number of spheres in

![Figure 1](image1.png)

**Figure 1.** (a) Schematic description of the experimental setup. (b) Top view (with the five measurement points. 104, 208, 312, 416 and 520 mm).

| Operation conditions | Air flow | Nitrogen flow |
|----------------------|----------|--------------|
| m\(^3\)h\(^{-1}\)   | Superficial Velocity (m\(\cdot\)s\(^{-1}\)) | Real velocity (m\(\cdot\)s\(^{-1}\)) | m\(^3\)h\(^{-1}\) | Velocity, m\(\cdot\)s\(^{-1}\) | Volume flow ratio |
| 40                   | 0.050    | 0.102        |              | 5          | –            | 12.5         | 4.5       | 0.125    |
| 83                   | 0.101    | 0.210        |              | 15         | –            | 37.0         | 13.5      | 0.375    |
| 150                  | 0.183    | 0.381        |              | 25         | –            | 62.4         | 22.4      | 0.625    |
| 250                  | 0.306    | 0.637        |              | 5          | 50           | 12.5         | 4.5       | 0.060    |
|                      |          |              |              | 15         | 150          | 37.0         | 13.5      | 0.180    |
|                      |          |              |              | 25         | –            | 62.4         | 22.4      | 0.300    |
|                      |          |              |              | 5          | 50           | 12.5         | 4.5       | 0.033    |
|                      |          |              |              | 15         | 150          | 37.0         | 13.5      | 0.099    |
|                      |          |              |              | 25         | –            | 62.4         | 22.4      | 0.166    |
|                      |          |              |              | 5          | –            | 12.5         | 4.5       | 0.020    |
|                      |          |              |              | 15         | –            | 37.0         | 13.5      | 0.060    |
|                      |          |              |              | 25         | –            | 62.4         | 22.4      | 0.100    |
the Z-direction (box height). Columns are in the cross flow direction (box length in the X-direction), whereas rows are in Y-direction (box width). The SC arrangement results in 11 layers with 7 columns and 12 rows of ceramic spheres for a total of 924 spheres which leads to a porosity of \( \varphi = 0.48 \).

The oxygen molar concentration was measured at different positions in the bed by using gas analyzer with an accuracy of ±0.2 vol. %, resolution of 0.01 vol. % and a response time of 20 sec. Measurements are carried out by sucking off a small amount of gas mixture through a lance slid vertically to the particle bed. Five measuring positions on the X-direction (0.104, 0.208, 0.312, 0.416 and 0.520 m) are applied as shown in Figure 1(b). The measurements were taken at a height of 0.468 m in Z-direction.

3. Computational fluid dynamics model

For the present study, the description of the CFD method with the equations for conservation of mass, momentum, and species was used. Turbulent flow is assumed for all runs due to high flow rates, leading to the Reynolds-averaged Navier–Stokes equations (RANS), which were then discretized by the finite volume method. The turbulence model used for enclosed domain was the \( \kappa - \varepsilon \) standard approach with standard wall functions. The detailed equations and background of these balances are mentioned in Fluent (2005) Users Guide version 6.2, and the numerical approach is described as follows:

3.1. Fixed bed model (FBM)

3.1.1. 3D model geometry

In the present study, a rectangular box was created to simulate the experimental test rig as shown in Figure 1(a). In order to reduce the effect of outlet boundary conditions an extra height of 50 mm was added to the main box. The aspect ratio (box equivalent diameter to particle diameter ratio) in this study is \( N = 9 \). The Solid Work version 2014 was used to draw the geometry while ANSYS 14 was used to analyze and generate mesh models for CFD. For mesh creation and further modifications, the geometry file should be exported as a file type of Parasolid to the ANSYS Design Modular.

3.1.2. Numerical approach

The CFD flow solver based on finite volume method is used in the present work to solve Reynolds-averaged Navier–Stokes (RANS) equations and species transport. The flow is assumed as steady and incompressible. The conservation equations of continuity and momentum can be represent as follow:

\[
\nabla \cdot (\rho \mathbf{U}) = 0 \tag{1}
\]

\[
\nabla \cdot (\rho \mathbf{UU}) = -\nabla p + \nabla \cdot [\mu_t(\nabla \mathbf{U} + \nabla \mathbf{U}^T)] \tag{2}
\]

where the turbulent viscosity is defined as:

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \tag{3}
\]

The standard \( \kappa - \varepsilon \) model was used in the present CFD work. The transport equations for the turbulent kinetic energy equation and the dissipation rate equation respectively are represent as follow [15]:

\[
- \nabla \cdot \left[ \left( \eta + \rho \frac{C_{\mu}k^2}{\sigma_k\varepsilon} \right) \nabla k \right] + \rho \mathbf{U} \cdot \nabla k = \rho C_{\mu} \frac{k^2}{\varepsilon} (\nabla \mathbf{U} + \nabla \mathbf{U}^T)^2 - \rho \tag{4}
\]

\[
- \nabla \cdot \left[ \left( \eta + \rho \frac{C_{\mu}k^2}{\sigma_k\varepsilon} \right) \nabla \varepsilon \right] + \rho \mathbf{U} \cdot \nabla \varepsilon = \rho C_{\varepsilon 1} C_{\mu} \kappa (\nabla \mathbf{U} + \nabla \mathbf{U}^T)^2 - \rho C_{\varepsilon 2} \frac{k^2}{\varepsilon} \tag{5}
\]

where, the turbulence model parameters (constants) are determined from experiments:

\[
C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92, C_{\mu} = 0.09, \sigma_k = 1.0, \sigma_\varepsilon = 1.3
\]

In addition, the mixing and transport of chemical species can be modeled by solving conservation equations describing convection, diffusion, and reaction sources for each component species. The general form of this conservation equation is as follows (Fluent, 2005):

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot \mathbf{J}_i + R_i + S_i \tag{6}
\]

where \( Y_i \) is the local mass fraction of each species, \( R_i \) is the net rate of production of species \( i \) by chemical reaction and \( S_i \) is the rate of creation by addition from the dispersed phase plus any user-defined sources, \( \mathbf{J}_i \) is the diffusion flux of species \( i \), which arises due to concentration gradients.

\[
\mathbf{J}_i = (\rho D_{i,m} + \frac{\mu_t}{S_{c_i}}) \nabla Y_i \tag{7}
\]

where \( D_{i,m} \) is the diffusion coefficient for species, \( i \) in the mixture, and \( S_{c_i} \) is the turbulent Schmidt number which defined as:

\[
S_{c_i} = \frac{\mu_t}{\rho D_i} \tag{8}
\]

where \( \mu_t \) is the turbulent viscosity and \( D_i \) is the turbulent diffusivity.
### 3.1.3. Contact points

Contact point problems or high skewed elements do not appear in the laminar flow (Calis et al., 2001). But when the flow is developing to turbulent the convergence solution is unachievable. This is due to the increasing of the flow velocities in the fluid element around the contact points. Thus, in this study, high Reynolds number (700 to 4400) were used which requires a turbulence model to simulate the test section in reality. Therefore, the new mathematical domain reduces the skewed element around the contact points by one of the three methods (gap, overlap, bridge) as shown in Figure 2. Those methods are studied by a lot of researchers (Calis et al., 2001; Dixon & Nijemeisland, 2001; Dixon, Nijemeisland, & Stitt, 2013; Eppinger et al., 2011; Guardo, Coussirat, Larrayoz, Recasens, & Egusquiza, 2004; Ookawara et al., 2007), but for pressure drop, heat transfer, and drag coefficient for axial flow, see Table 2. The present study also used these methods but for cross flow mixing through the packed bed to investigate which method can be adopted by validating CFD results with experiment data. The 1 mm space between the spherical particles in the mathematical model was chosen depending on previous research conducted by Calis et al. (2001). The choice of this space made our model closed to the real domain porosity as shown in Table 2. Therefore, adopting 1 mm of particle Spacing/Overlapping distance at contact points will result in increasing/reduction of the computational domain dimension of the gap/overlap model respectively, Table 3. The bridge model is generated by creating a cylinder connection between particle-particle and particle-wall with a radius $= 0.1d_p$ (particle diameter). Those cylinders will remove the fluid in the narrow gap surrounding the contact point, and it should be meshed these cylinders or bridges together with the particles (spheres), the mesh size in this method has doubled in comparison to the other two methods, and the porosity will be 0.4769. Table 3 explains the dimensions for each method. Those three methods ensure reduced high skewed elements in the near wall contact points.

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#### Table 2. Contact point studies.

| Name & Year          | Contact point treatment | Field                        | No. of particle |
|----------------------|-------------------------|------------------------------|-----------------|
| Calis et al. (2001)  | Gap                     | Pressure drop, fluid flow    | 16              |
| Dixon & Nijemeisland (2001) | Overlap               | Pressure drop, heat transfer | 44              |
| Guardo et al. (2004) | Bridge                  | Pressure drop, temperature distribution | 240 to 880 |
| Ookawara et al. (2007) | Caps                   | Pressure drop, velocity distribution | 80 to 750 |
| Eppinger et al. (2011) | Caps                   |                              |                 |

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**Figure 2.** (a) Three methods for contact point treatment. (b) Histograms distribution of the cell equivolume skew and $y^+$ values for the wall region.
Table 3. Computational domain dimensions.

| Test section | SC Bed dimensions (m) | Real dimensions (m) | gap | Overlap | bridge |
|--------------|-----------------------|---------------------|-----|---------|--------|
|              |                       | L                   | 0.624 | 0.637   | 0.611  | 0.624 |
|              |                       | W                   | 0.364 | 0.372   | 0.356  | 0.364 |
|              |                       | H                   | 0.572 | 0.584   | 0.560  | 0.572 |
| Volume (m³) |                       |                     | 0.1299 | 0.1388  | 0.1218 | 0.1299 |
| Porosity ϕ  |                       |                     | 0.48  | 0.5083  | 0.4417 | 0.4769 |

3.1.4. Turbulence model and boundary conditions

According to the porous flow in general, the distinct flow regimes are largely determined by the particle Reynolds number, namely: Darcy flow (Reₚ < 1), Forchheimer flow (1–10 < Reₚ < 150), unsteady flow (150 < Reₚ < 300), fully turbulent flow (Reₚ > 300) (Unaspekov & Strekalova, 2002).

In the present study, the Reynolds number for the main flow of air varied from (700 to 4400) and for the crossflow of nitrogen from (2000 to 60000) which leads to turbulent flow due to high resistance at air flow inlet through 66 holes in the perforated plate. The two inlet velocities vary depending on flow rate values for both air and nitrogen. The inlet boundary conditions are shown in Table 4. For complex flow, the κ–ε turbulence model has long been popular. The standard κ–ε model is widely used in the industrial flow problems because of it is economical and high accuracy, the standard κ–ε turbulence model and species transport model were employed for all simulations to calculate the O₂ concentration as a result of cross flow mixing between air and nitrogen. The fluids were taken to be incompressible with a temperature of 300 K. First order upwind schemes were selected to compute the field variables because second order upwind are difficult to converge due to complex geometry used in this study. The pressure-velocity coupling algorithm was the SIMPLE (Semi-Implicit-method for Pressure Linked Equations) scheme, and all under-relaxation factors are set as a default except momentum in 0.5. The turbulent intensity for all runs is 5%.

Table 4. Inlet and outlet boundary conditions.

| boundary | Dn, m | Flow rate (m³ h⁻¹) | Temperature (k) | Turbulent Intensity (l) |
|----------|-------|-------------------|----------------|-------------------------|
| inlet air | 66*20 | 40,83,150,250      | 300            | 0.05                    |
| N₂       | 6,12,20 | 5,15,25          | 300            | 0.05                    |
| outlet   | 0.459 | –                 | 300            | 0.05                    |

3.1.5. Mesh study and domain meshing

In order to calculate the concentration of gas mixing through the bed, the mesh must be fine enough for more accurate of solution: Figure 3(a). Therefore, it is important and necessary to conduct a mesh independence study, by increasing the number of mesh elements and monitoring the velocity and pressure drop in such height in the bed. Figure 3(b) explain a series of mesh sizes, from coarsest with mesh 29 cells/cm³ to finest mesh with 401 cells/cm³ are created, as shown in Table 5. The computational results show that the solution of the flow velocity becomes grid independent after two levels coarsest to the finest grid. The mesh type on the particle surface, which indicates the grid structure of the whole domain. As can be noted, the grid is fine in the small gaps and becomes coarser in the larger void area. The mesh creation for mesh study and the computational domains was done by using the workbench. Therefore, the simplest method for mesh generating was adapted. Patch conforming tetra meshing method was selected. Although

Figure 3. (a) Computational mesh geometry with 1mm interval size. (b) Five grade of interval size for mesh.
Table 5. The grid used for grid convergence study and computational results (\(U_{\text{air}} = 3.35 \text{ m.s}^{-1}\) \(U_{\text{N}_2} = 22.5 \text{ m.s}^{-1}\), for FBM gap method).

| Grid     | Interval size | Cells       | Density Cell/cm\(^3\) | \(Y^+\) average | Pressure Pa at plane \(Z = 0.468\) | Velocity m/s at plane \(Z = 0.468\) | CPU time Min |
|----------|---------------|-------------|------------------------|------------------|----------------------------------|----------------------------------|--------------|
| mesh 1   | 5             | 1,221,675   | 29                     | 7.03             | 0.560                            | 0.633                            | 35           |
| mesh 2   | 3             | 2,391,425   | 58                     | 6.07             | 0.618                            | 0.657                            | 69           |
| mesh 3   | 1             | 4,642,931   | 111                    | 4.70             | 0.650                            | 0.657                            | 240          |
| mesh 4   | 0.8           | 7,606,744   | 182                    | 4.40             | 0.668                            | 0.660                            | 420          |
| mesh 5   | 0.5           | 16,699,809  | 401                    | 3.80             | 0.690                            | 0.659                            | 1275         |

Table 6. Mesh element and computing time.

| Case        | Sphere diameter (mm) | Pitch (mm) | Number of elements | CPU time (hours) |
|-------------|-----------------------|------------|--------------------|------------------|
| FBM (\(\varphi = 0.48\)) gap | 52 | 53 | 6,643,000 | 7 |
| FBM (\(\varphi = 0.48\)) overlap | 51 | 51 | 6,255,000 | 6 |
| PMM (\(\varphi = 0.48\)) Bridge | 52 | 52 | 9,629,000 | 12 |
| PMM (\(\varphi = 0.48\)) | 52 | | 881,205 | 1/2 |

this method is fully automated, it has additional mesh controls and capabilities. In order to control the mesh size, the body size option was used to specify the element size used for the entire model. The domain typically was meshed at the cell size of \(dp/52\). Figure 2(b) demonstrates that the mesh contains a few highly skewed elements, most of the skewed elements are located in areas of a particle near contact points. And the \(y^+\) values near the solid wall (spheres wall). The \(y^+\) is a non-dimensional distance value and it is important in turbulence modeling to determine the proper size of the cells near walls (Fluent, 2005). In the present study, it is less than 5 at the surface of spheres and walls. Table 6 shows the total number of mesh elements and the CPU timing for the three methods of contact point treatment. All simulations in the present work applied the 1 mm interval size for mesh generation. The simulations presented in this work have been performed on (Intel Core (TM) i5 four core 3.1 GHz PC).

3.2. Porous media model (PMM)

According to the difficulties in FBM for dealing with contact points in a real box, another approach (PMM) has been used. Actually, constructing the geometry is easily in case of PMM rather than FBM. Wu and Ferng (2010) reported that, the porous media approach for closely packed geometry can help a CFD simulation to quickly and reasonably capture the averaged behaviors of the thermal-hydraulic parameters. The computational time in case of PMM is very small compared to FBM. In porous media model the geometry can easily be created by substituting the spheres resistance by a resistance source to the momentum equation to get the same particle effect and hence has great limitations in application. Besides, there are some restrictions placed upon the geometry of the porous media (Yang et al., 2010). Then the grids were created with tetrahedral in the porous zone and the rest of the upper part of the computational domain is meshed with hexahedral. Mesh independence of the simulation results are obtained by a variation of the number of mesh elements, the model strategy is deployed again in order to reduce the computational effort. The half of the test box geometry consists of the main flow (air) inlet from bottom, and second inlet for injection flow (\(N_2\)) indicated by the lance, a mixture outlet, and symmetry plane (Figure 4). The mesh has 881,205 cells in all: see Table 7.

3.2.1. Governing equations

In this section, the governing equations for fluid flow and heat transport through porous media will be introduced. As we know, porous media are modeled by the addition of a momentum source term to the standard fluid flow equations. The source term is composed of two parts: a viscous loss term (Darcy, the first term on the right-hand side of Eq. 9), and an inertial loss term (the second term on the right-hand side of Eq. 9) (Fluent, 2005).

\[
S_i = - \left( \sum_{j=1}^{3} D_{ij} \mu v_j + \sum_{j=1}^{3} C_{ij} \frac{1}{2} \rho |v| v_j \right) \quad (9)
\]

where \(S_i\) is the source term for the \(i\)th \((x, y, \text{ or } z)\) momentum equation, \(|v|\) is the magnitude of the velocity and \(D\) and \(C\) are prescribed matrices. This momentum sink contributes to the pressure gradient in the porous cell, creating a pressure drop that is proportional to the fluid velocity (or velocity squared) in the cell. In the case of simple homogeneous porous media (isotropic media), it can be written as

\[
S_i = - \left( \frac{\mu}{\alpha} v_i + C_2 \frac{1}{2} \rho |v| v_i \right) \quad (10)
\]
Figure 4. Geometry and computational mesh for the PMM.

Table 7. Values for the viscous and inertial resistance coefficients relative to the porosity.

| Porosity | Viscous resistance (m$^{-2}$) | Inertial resistance (m$^{-1}$) |
|----------|-----------------------------|-----------------------------|
| 0.35     | 546647                      | 1020                        |
| 0.48     | 135633                      | 316                         |
| 0.60     | 41091                       | 124                         |
| 0.70     | 14555                       | 58                          |
| 0.80     | 4333                        | 26                          |

Or written as the pressure drop per unit length

$$\frac{\Delta P}{L} = -\left(\frac{\mu}{\alpha}v_i + C_2 \frac{1}{2} \rho |v| v_i\right)$$  \hspace{1cm} (11)

where $\alpha$ is the permeability and $C_2$ is the inertial resistance factor. To model a porous region without considering heat transfer, the main additional inputs for the problem setup are defining the porous zone and specifying the porosity of the porous medium, and setting the viscous resistance coefficient $1/\alpha$ and the inertial resistance coefficient $C_2$. As the porosity is known, to find the resistance coefficients is hence the first task. Methods for determining the permeability and the inertial resistance factor are presented below.

3.2.2. Using the Ergun equation for a packed bed

Considering the modeling of a packed bed, the appropriate constants can be derived by using the Ergun equation, a semi-empirical correlation applicable for many types of packing:

$$\frac{\Delta P}{L} = 150. \frac{(1 - \varphi)^2}{\varphi^3} \mu \frac{U}{dp^2} + 1.75 \frac{1 - \varphi}{\varphi^3} \rho \frac{U^2}{dp}$$  \hspace{1cm} (12)

where $dp$ is the mean diameter.

Comparing Eq. 9 with 11, the permeability and inertial loss coefficient in each component direction can be identified as

$$\alpha = \frac{dp^2 \varphi^3}{150(1 - \varphi)^2}$$  \hspace{1cm} (13)

and

$$C_2 = \frac{(1 - \varphi)}{dp \varphi^3}$$  \hspace{1cm} (14)

As can be observed in Eq. 13 and 14, both coefficients are determined by the geometry parameters.

3.2.3. Superficial velocity

The carriage of flow through a porous medium obeys the same relationships as for basic fluid mechanics. The volume of fluid per unit time or fluid flux transported through the bed is described by the volumetric flow rate, $Q$ (m$^3$/s). This is related to the superficial velocity, $U$, from simple dimensional reasoning in the form of:

$$U = \frac{Q}{A}$$  \hspace{1cm} (15)

where $A$ (m$^2$) is the cross sectional area of the tube. The superficial velocity the velocity that would be present in the absence of the media. For instance, a flow measuring device placed immediately before the media would measure the superficial velocity.

Another term to used to describe the velocity is the interstitial velocity, $U_i$, which is the average velocity within the pores. This takes into account the bed porosity through
the relation
\[ U_i = \frac{U}{\varphi} \]  \hspace{1cm} (16)

where \( \varphi \) is the porosity.

The resistance coefficients are computed based on different porosities for ceramic sphere diameter of 52 mm, as shown in Table 6.

4. Results and discussion

The main purpose of the CFD simulations were to test its capabilities to simulate the cross flow mixing in simple cubic packed beds. The CFD simulations results are presented in the form of \( O_2 \) molar concentration contour plots and curves. The following results are for the comparison between the CFD simulation and experimental measurements.

4.1. Studied method (contact point treatment)

Figure 5 shows the comparison between the simulation results of the three methods of FBM and the measurement data at level \( Z = 0.468 \text{ m} \) (more than 8 times of sphere diameter higher than the injection position), the injection position \( X_L = 0.156 \text{ m} \) and lance diameter is \( d_L = 0.02 \text{ m} \). The figure demonstrates that the three methods nearly have the similar profile. But, the gap method is much closer to the experimental data, especially with high volume flow rate ratio \( (V_R = 0.625) \). The error between the CFD results and experimental data is ranged from 7 to 18\%, 10 to 25\% and 2 to 26\% for the gap, overlap and bridge respectively. Referring to Table 6, the time consumed in the bridge method is larger than for gap and overlap. Therefore, from the figure, the gap method is recommended when comparing the CFD results with the experimental data as will be described in the following section.

4.2. Volume flow rate ratio

The effect of the volume flow rate ratio on the oxygen concentration is shown in Figure 6 for the three methods. The air flow is the parameter while the \( N_2 \) flow is constant at 25 \text{ m}^3\cdot\text{h}^{-1}. The first figure represents the comparison

![Figure 5](image1)

*Figure 5. Comparison of the three methods for FBM and experimental data, at \( X_L = 0.156 \text{ m}, d_L = 0.02 \text{ m} \).*

![Figure 6](image2)

*Figure 6. CFD results of \( O_2 \) concentration for FBM and experimental data for different \( V_R \) and the Contours plots of gap method, at \( X_L = 0.156 \text{ m}, d_L = 0.02 \text{ m} \).*
between the CFD results and the experimental data. The figure demonstrates that for low volume flow rate ratios the O₂ concentration decreases till the middle of the box then it increases again until O₂ concentration reaches 21% at the end of the box. The minimum in all profiles can be defined as the penetration depth of the jet. This means that the mixing of the two flow streams is weak. But, by increasing the volume ratio, the curve looks like a flat curve till the position of 0.5 m. As a consequently, the mixing between the two streams is good. Furthermore, the CFD results are fitted well with the experimental data for all volume ratios. Moreover, the figure represents the contour plots. From these contour plots when the volume flow rate ratio decreases, more oxygen is spread in the bed. Generally, it can be concluded that for higher volume flow rate ratio the CFD results are best fitted with the experimental data.

4.3. PMM & FBM

Figure 7 represents a comparison between the CFD calculations for FBM (gap method) with porosity 0.48, and the PMM with the same porosity for volume ratio \( V_R = 0.06 \) at \( X_L = 0.156 \) m and \( d_L = 0.02 \) m. In addition, the figure shows the contour plots of FBM and PMM at inlet, outlet, and symmetry planes. Figure 7 shows that the O₂ concentration curve for FBM (gap method) are fit better with the experiments than that from PMM. The figure demonstrates that there are a deviations between the PMM results and FBM results. One of these limitations is that the ANSYS FLUENT uses the superficial velocity inside the porous medium model, based on the volumetric flow rate, to ensure continuity of the velocity vectors across the porous medium interface. This velocity is far from the realistic case. The other limitation

![Figure 7](image1.png)

**Figure 7.** Comparison of the O₂ concentration between CFD results (FBM gap method and PMM at the same porosity) and the experimental data, at \( X_L = 0.156 \) m, \( d_L = 0.02 \) m.

![Figure 8](image2.png)

**Figure 8.** (a) Effect of the lance injection depth on the O₂ concentration; (b) Contour of O₂ concentration at ZX (symmetry) planes by FBM, \( d_L = 0.02 \) mm.
is related to the effect of the porous medium on the turbulence field which is only approximated.

4.4. Lance position (injection position)

Figure 8 shows the effect of lance position on the O₂ concentration for volume ratio $V_R = 0.06$ with respect to the experiment data. In addition, the contour plots for the three different injection positions are represented. In the figure, the two injection positions 0.156 and 0.312 m were shifted to the position of 0 m. So that, the injection always starts at 0 m. The figure demonstrates that all profiles fell together and forms a jet of N₂. The injection position of 0.312 m formed the left side of the jet and the injection position of 0 m the right side. Therefore, it can be concluded that the shape of the jet is independent of the injection position. Furthermore, the figures show that the FBM gap method simulation results have a good agreement with the experimental data.

4.5. Lance diameter (injection velocity)

Three lance diameters (6, 12, and 20 mm) have been studied to show the effect of the injection velocity on the O₂ concentration. Figure 9 demonstrates that at $V_R = 0.625$ (high value) the O₂ concentration curve for all lance diameters appears to be constant for both experiments and simulations. While at low $V_R = 0.06$ the O₂ concentration curves forms an inverted bell shape distribution. This means the distribution in the bed is not good at low flow rate ratio. The results revealed that the lance diameter (injection velocity) has low effect on flow mixing in the packed bed on the contrary of the lance behavior in empty bed [33].
4.6. Velocity profiles

Figure 10 represents the velocity distribution of the six lines, see Figure 1(b), with 11 points per line, every sphere. The velocity measurements were done by using a hot wire with an error of about \( \pm 0.01 \text{ m} \cdot \text{s}^{-1} \). Actually, there were some problems in obtaining the absolute velocity during the measurements. These problems were related to the human error in hot wire fixation, but the tendency of the distribution is acceptable. From the figure, it can be concluded that there is no difference in the mixing velocity distribution through the cross lines at the outlet of the box. Therefore, we conduct all the results at line 3. Also, the results obtained from the CFD simulations were taken from the same line.

Figure 11 shows the mixing velocity distribution for a volume flow rate ratio of 1.25 with injection position of 0.156 m. From the figure the CFD results have the same trends, and much fitted with the experimental data after the injection position. Actually, the peaks in the simulation results represent the velocity. Regarding the experimental data, the figure showed that the average of the mixing velocity at the outlet was 0.85 and. But for the simulated results, the average of the mixing velocity was nearly half that of the experimental.

Figure 12 presents the velocity magnitude contours in the plane at the lance level \( Z = 0.026 \text{ m} \) and at the outlet plan at \( Z = 0.57 \text{ m} \), for PMM and FBM. It can be seen that the velocity is decelerated sharply for PMM, the main reason is the superficial velocity values within a porous region remain the same as those outside the porous region, and it cannot predict the velocity increase in porous zones and thus limits the accuracy of the model.

5. Conclusions

In this paper the gas cross flow mixing in structured packed beds was simulated for a simple cubic packing. The influence of these parameters (methods of contact point treatment, volume flow rate ratio, porous media model, lance position and lance diameter) on the cross flow mixing are studied with CFD simulation and the results are compared to experimental data. From the reported results, the following conclusions are drawn:

- The CFD simulation can predict the cross flow mixing in the structured packed bed by using \( \text{O}_2 \) molar concentration as a new method for data reporting.
- The model with the gap method generates the best results of oxygen molar concentration compared to the experimental results.
- As the volume flow rate decreases the agreement between CFD simulations and experimental data is very satisfactory.
- The injection position has a great influence on the oxygen concentration profiles in the bed.
- The jet penetration and widths only depend on the ratios of the two flows, not on their absolute value.
- The shape of the jet is independent of the location of injection.
- The results show that by using the porous media model the number of grids and computation time can be decreased.

Nomenclature

| Symbol | Description | Unit |
|--------|-------------|------|
| \( B \) | Width       | m    |
| \( d_p \) | Particle diameter | m    |
\[d_L = \text{Lance diameter}\]

\[I = \text{Turbulent intensity, } 0.16(\text{Re}^{-0.125})\]

\[L = \text{Length}\]

\[N = \text{box equivalent diameter to particle diameter ratio}\]

\[\text{Re} = \text{Reynolds number}\]

\[U = \text{Velocity}\]

\[V_{ax} = \text{Air axial flow rate}\]

\[V_i = \text{N}_2 \text{ injection flow rate}\]

\[V_R = \text{N}_2 \text{ to air flow ratio}\]

\[X_L = \text{Lance depth in X direction}\]

\[\psi = \text{Porosity}\]

\[\mu = \text{Dynamic viscosity}\]

\[\rho = \text{Density}\]

Abbreviations

CFD: Computational fluid dynamics

FBM: Fixed bed model

PMM: Porous media model

SC: Simple cubic

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