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CFD ANALYSIS OF CATALYST SHAPE EFFECTS ON HYDRODYNAMIC AND HEAT TRANSFER CHARACTERISTICS OF FIXED BED REACTORS

Yaghoub Behjat, Afshin Ziyari, Majid Kakavand

Process Development and Equipment Technology Division, Research Institute of Petroleum Industry, Tehran, Iran

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Abstract

In this research, the effects of cylindrical catalyst shape on hydrodynamic and heat transfer characteristics of fixed bed reactors have been investigated by means of CFD analysis. In the developed model, the catalyst particles have been considered as porous media whose thermal conductivity are associated with the heat transfer from the reactor wall to bed. The computational model was validated using corresponding experimental data to predict the spherical catalyst heat transfer rate to the bed center. Comparison between the CFD model results with experimental radial temperature profile reveals that the computational model is able to predict the rate of the heat transfer with acceptable accuracy. The validated computational model has then been used to investigate the effects of ten types of cylindrical catalyst shapes on hydrodynamic and heat transfer characteristics of a fixed bed reactor with bed-to-particle diameter ratio (N) of 2 and 4. The results obtained from the CFD model indicate that due to the catalysts configuration and their contact points, there would be a complicated flow field around the catalysts. Comparing the bed heat transfer and pressure drop amounts for two cases (N=2 and 4) indicates that the optimum catalyst shape for increasing the heat transfer ratio to the bed center and lowering the pressure drop along the bed for the two cases (N= 2 and 4) is the same. On the other hand, CFD simulation results show that increase of the number of the holes in catalysts considerably decreases the bed pressure drop, while it has a minor effect on decreasing the heat transfer rate to the bed center.

Keywords: *Fixed Bed Reactor; Hydrodynamic; Heat Transfer; Catalyst Shape; CFD Simulation.*

1. Introduction

Catalysts with complex shapes such as punching tablets are widely used in industrial steam reforming processes. Formed catalysts are used to increase the effective mass transfer, increase the heat transfer and decrease the pressure drop. Although simulation of the steam reforming process by means of one-dimensional and two-dimensional models have been widely reported in the literature but optimization of the catalysts dimensions and shapes, as well as development of certain relations for prediction of heat transfer characteristics, have been little cited. Researches on CFD simulation of fixed bed reactors have been generally done by limited research groups, mainly focusing on the rate of heat transfer in these beds.

Dixon and his colleagues in their first research activities in this field determined the turbulence model as well as the required parameters for CFD simulation of fixed bed reactors by means of some simple experiments. Their experiment was an investigation of the heat transfer amount to a column having a diameter of 2 inches and a length of 18 inches with boundary condition of a steady temperature at the walls. In this bed, spherical catalysts with a diameter of 1 inch had been used [1].

Some other researchers simulated the system with different shape of catalysts to study the effects of catalyst shapes on the hydrodynamic and heat transfer characteristics of the bed. The main goal of these simulations was to investigate the effects of the catalyst shape on the

heat transfer characteristics near the walls and also study the influence of the catalyst holes and empty spaces on the heat transfer. The results of these simulations showed that the shape of the catalyst has a minor impact on the heat transfer near the walls, but in the bed center it has a major influence. The reported results showed that under a steady pressure drop the temperature of the reactor and walls increases if non-porous catalysts are applied [2].

Dixon and his colleagues in the second stage of their researches simulated the effects of the catalyst shape on the reaction inside the bed. This study was done with a spherical catalyst. The results indicated that the assumption of steady temperature and steady catalyst particle concentration will remain satisfied for catalyst particles far from the walls, but for those near the walls, it will be violated. With no more simulations, they concluded that the same results will be maintained for non-spherical catalysts [3].

In their third research activities, Dixon and his colleagues investigated the effects of catalysts shape on the pressure drop and heat transfer in fixed bed reactors. In this research 5 different catalyst shapes were simulated with the bed by means of CFD. The results showed that the cylindrical catalyst with 4 holes yields the minimum pressure drop and heat transfer ratio. The filled catalyst (without holes) particles resulted in maximum pressure drop and heat transfer ratio. In this study, the effects of the catalyst thermal conductivity have not been investigated [4].

Guardo and his colleagues investigated the effects of the turbulence model in CFD analysis of the fixed beds in their first research work. In this study turbulence models with one and two equations models have been applied and the pressure drop value deducted from the simulation has been compared with experimental and semi-experimental data. In all simulated cases, canalization has occurred near the walls and in the empty spaces of the catalyst particles. All the results of these simulations have been compatible with those of the magnetic photography experiments [5]. In their second research works, Guardo and his colleagues have investigated the effects of the heat transfer from the fluid to the catalyst particles. In this work, the heat transfer coefficient between the gas and the catalyst particles inside the bed has been computed. It is observed that adequate mesh has not been considered in the contact points of the catalysts which have resulted in a considerable error in the numerical solution of the equations [6].

Heat transfer of single cylindrical particle affected by wall has been investigated numerically and experimentally for limited Reynolds number. The heat transfer in two different orientations (axial and cross flow over the particle) considered by Hashemabadi *et al.* Influence of wall on heat transfer of particle in different bed-to-cylinder diameter ratio discussed [7]. Hashemabadi *et al.* studied experimentally and computationally the flow and heat transfer characteristics of regularly arranged cylindrical particles in a bed with a bed-to-particle diameter ratio of 2.65 in two different arrangements of particles [8]. Hashemabadi et al. in the other research investigated numerically and experimentally the heat transfer of a multi-lobe particle (tri-lobe, tetra-lobe, and penta-lobe) affected by the wall in cross and axial-flow was. The heat and mass transfer analogy was applied for gaining the Nusselt number for each particle in axial and cross flow [9].

In literature, minor attention has been paid to the shape of catalysts, and they have usually been considered to be spherical in simulations. Also, the effects of catalyst shapes on hydrodynamic and heat transfer characteristics have not yet been studied comprehensively with precise optimum computational grids. In this research, the effects of catalyst shapes on hydrodynamic and heat transfer characteristics for a fixed bed reactor with bed-to-catalyst particle ratio of 2 has been studied. In addition to the spherical catalyst, 10 different cylindrical catalyst shapes with bed-to-catalyst particle ratio of 2 and 4 have been also incorporated in CFD simulations to be studied for their effects on the hydrodynamic and temperature profile inside the bed.

2. Governing equations and modeling

The general form of the equation used for mass conservation law (continuity equation) is as follows [2,10,11]:

$$\frac{\partial \rho}{\partial t} + \nabla.\left(\rho\, \vec{v}\right) = 0 \quad (1)$$

Momentum and energy conservation equations are as followings:

$$\frac{\partial}{\partial t}\rho\, \vec{v} + \nabla.\left(\rho\, \vec{v}\, \vec{v}\right) = -\nabla P + \rho g + \nabla.\overline{S} + S_i \quad (2)$$

$$\rho C_P\left(\frac{\partial}{\partial t}T + \vec{v}\,.\nabla T\right) = -\nabla.\left(k_{eff}\nabla T\right) \quad (3)$$

Turbulence equations are also incorporated in the computational model as the velocity of the gas phase in industrial steam reforming process is very high (Reynolds number = 25000). RNG k-ε turbulence model has been incorporated as it can be used to analyze swirl flows as well as the flows on high curvature surfaces because of the additional terms it has got in ε equation. Also for modeling of the turbulence near the reactor walls, the standard wall function model has been used [12-13].

$$\rho\frac{\partial k}{\partial t} + \rho v k = \left(\mu + \frac{\mu_t}{\sigma_k}k_j\right) + G - \rho\varepsilon \quad (4)$$

$$\rho\frac{\partial \varepsilon}{\partial t} + \rho v \varepsilon_j = \left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\varepsilon_j\right) + C_1\frac{\varepsilon}{k}G - C_2\rho\frac{\varepsilon^2}{k} - \frac{C_\mu\eta^3\left(1-{}^{\eta}/_{\eta_0}\right)}{1+\beta\eta^3}\frac{\varepsilon^2}{k} \quad (5)$$

In this research, the heat transfer phenomena inside catalyst particles have been simulated considering each catalyst particle as porous media. Porous media modeling includes experimental determination of flow resistance. Porous media is simulated by adding a momentum well to the standard flow field equation. This momentum includes viscous and inertial resistance as indicated in the following equation [10].

$$\mathrm{S_i} = -\left(\sum_{\mathrm{j=1}}^{3}\mathrm{D_{ij}}\mu\,\upsilon_\mathrm{j} + \sum_{\mathrm{j=1}}^{3}\mathrm{C_{ij}}\frac{1}{2}\rho|\upsilon|\upsilon_\mathrm{j}\right) \quad (6)$$

$\mathrm{S_i}$ is the cumulative momentum for part i (x,y) of momentum equation, $|\upsilon|$ is the velocity order and C and D are some defined matrixes. This momentum well is the cause of pressure gradient and accordingly a pressure drop proportional to fluid velocity (velocity into power 4) in a porous cell. For a homogenous porous medium we have:

$$\mathrm{S_i} = -\left(\frac{\mu}{\alpha}\upsilon_\mathrm{i} + \beta\frac{1}{2}\rho|\upsilon|\upsilon_\mathrm{i}\right) \quad (7)$$

where α is the permeability and β is the inertial resistance coefficient. For a slow flow in a porous medium, the pressure drop is usually proportional to velocity. Pressure drop in all directions (x,y,z) derived using the following relation:

$$\Delta\mathrm{p_i} = \sum_{\mathrm{j=1}}^{3}\frac{\mu}{\alpha_\mathrm{ij}}\upsilon_\mathrm{j}\Delta\,\mathrm{n_i} \quad (8)$$

Permeability and inertial resistance in relation (7) can be computed using the following equations:

$$\alpha = \frac{\mathrm{d^2_m}}{150}\frac{\phi^3}{(1-\phi)^2} \quad (9)$$

$$\beta = \frac{3.5}{\mathrm{d_m}}\frac{(1-\phi)}{\phi^3} \quad (10)$$

Pore size distribution (d_m) in the catalyst particles whose mean value has been considered 3792 Angstrom has been adopted from experimental data. Considering the pore size and the volume fraction of the catalyst particles because of the porous medium, β and $1/\alpha$ are computed as $\beta = 40562086.37$ and $\frac{1}{\alpha} = 2.34572 \times 10^{15}$ respectively.

3. CFD simulation

To generate an adequate geometry for the simulations, different shapes of the catalyst have to be randomly placed in the reactor. The main issue is to place the catalyst in the reactor in a manner to firstly avoid flow canalization and secondly produce a high quality mesh in the contact point of catalyst particles with each other and with the reactor wall. If the catalysts are tangent, it would be impossible to generate an adequate computational grid in contact points, and so the following approaches have been proposed for generating the required geometry.

- The catalyst particles volumes become greater up to the point that the contact point between them becomes a circle with a very small radius.
- The catalyst particles volumes become smaller up to the point that the contact point between them makes a small space in which suitable grids can be generated. It shall be noted that the catalyst sizes shall not be so much small to let the fluid flow between their contact points.

Considering that in this research the heat transfer is modeled as the thermal conductivity of the catalyst particles, an increase of particles volumes will cause the formation of an integrated catalyst volume inside the bed and hence increases the error. The increase of catalyst volume is not an adequate approach for generating a proper geometry. Accordingly, it was found better to reduce the catalyst volumes whose main challenging issue is the selection of the proper amount of this reduction. The decrease of catalyst volumes shall be up to a point to firstly avoid the flow of the fluid between the contact points and secondly increase considerably the amount of computation volume. It was found that a reduction of more than 1% in catalyst particles radiuses will cause a flow of the fluid between the contact points. The particles radiuses were decreased by 0.5%, and the simulations were carried out. The results showed that with this amount of catalyst volume reduction, no fluid will flow between the contact points of catalyst particles even up to Reynolds number of 70000.

To validate the computational model, an experimental bed with spherical catalyst was implemented using available experimental geometry and computational mesh data [1]. In this stage, the complete 360 degrees of the bed geometry was implemented, and the optimum computational grid was achieved for catalyst particles inner parts and surrounding fluid flow. The implemented bed contained 44 catalyst particles in 22 layers. The diameter of the bed was 2 inches while that of the catalyst particles was 1 inch. The center to center distance between two adjacent catalysts along the bed axis was$\sqrt{2}R$. So for placing the catalysts inside the bed, the catalysts of each layer are placed at a distance of$\sqrt{2}R$ long the bed axis from the previous layer and each layer is rotated 90 degree about the bed axis. The computational grid in this simulation is tetragonal which has been selected because of its geometry complexity. At least two computation cells have been considered in contact points of the catalysts with each other and with the reactor walls. Figure (1) illustrates the achieved computational grid of this bed with spherical catalysts. Figure (2) depicts 10 different cylindrical catalysts which have been simulated in this study.

Because of the catalysts random arrangement in the bed and hence the implementation of complex geometry, development of a proper computational cell in contact points of the catalyst particles is very difficult and time-consuming. Table (1) shows the boundary conditions of the achieved simulation.

Table 1. Boundary conditions of the simulated bed

Input, Velocity Constant	Velocity=14.3m/s, Temperature=600K, Turbulence=10%
Wall	No Fluid Slip, Temperature=1000K
Output	Constant Pressure

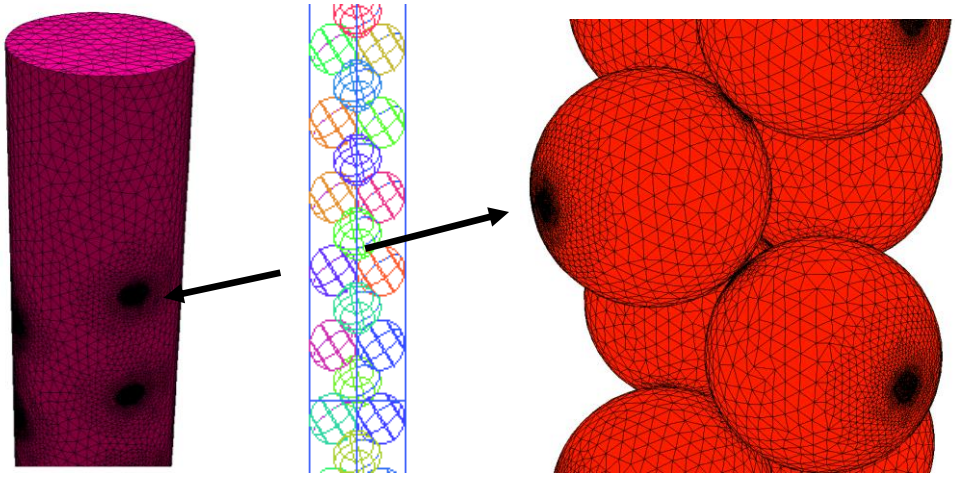


Figure 1. Schematic of the computational grid used for a bed with spherical catalysts

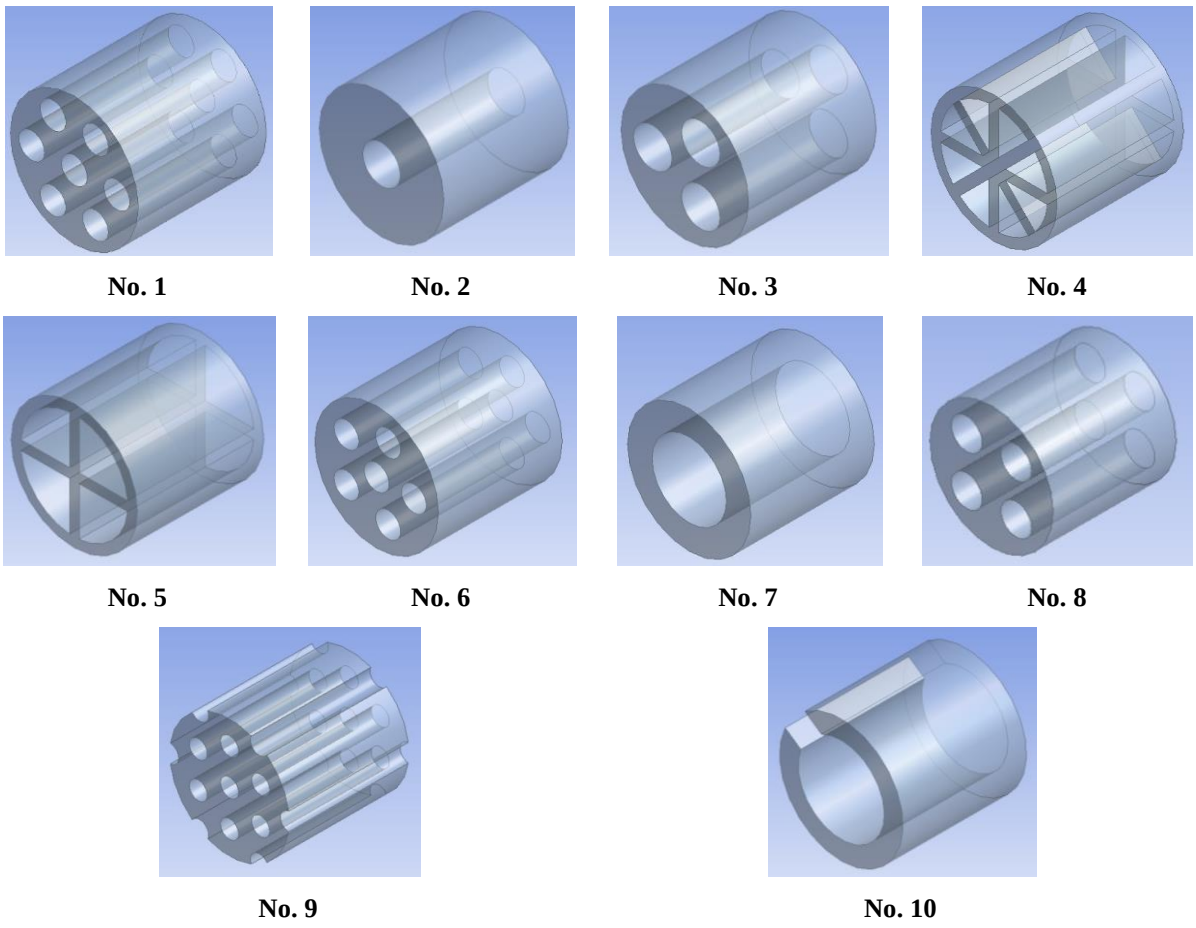


Figure 2. Ten different shapes of simulate cylindrical catalysts

Considering that the arrangement of the cylindrical catalysts inside the bed cannot be easily predicted and taking into account that this arrangement can extremely influence the results, it was decided to use two glass cylinders with internal diameters of 2 and 4 inches and cylindrical catalysts with diameter and height of 1 inch. For the bed with a bed to catalyst diameter ratio of 2, 10 pieces of catalysts were randomly placed in the glass cylinder of 2 inch diameter. Then geometry similar to the implemented bed was developed, and the meshing of the inner

parts of the catalysts, as well as the catalyst particle surrounding fluid flow, was achieved. Figure (3) illustrates the real bed, implemented bed geometry and developed computational grids for three types of catalysts (No. 3, No. 4, No. 9) for a bed with a bed to catalyst diameter ratio of 2 (N=2).

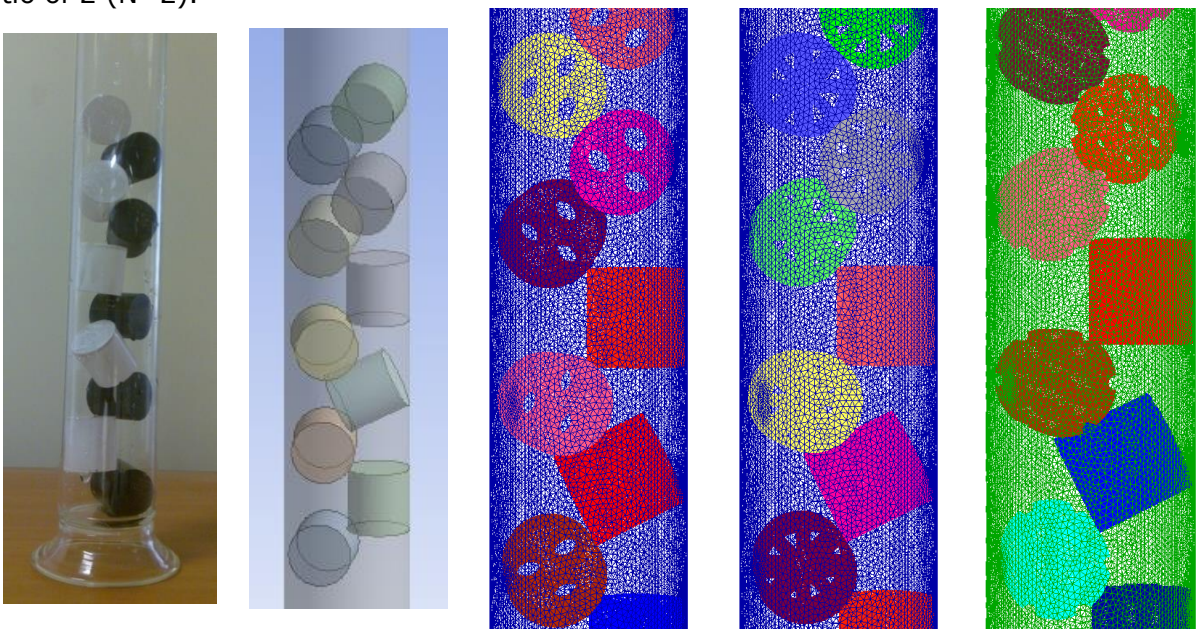
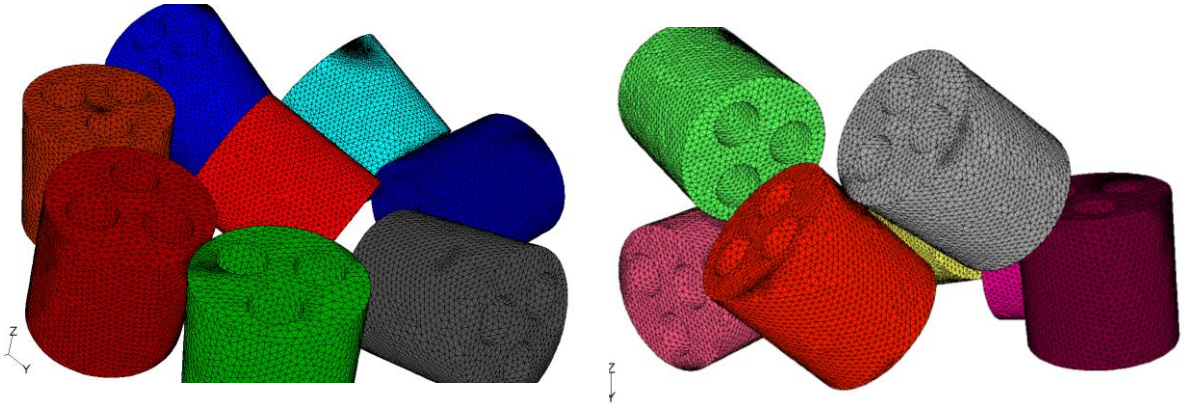


Figure 3. Real bed, catalysts geometry and developed grids for some catalysts

In next step, catalysts geometry was developed for a bed with a bed-to-catalyst diameter ratio of 4 (N=4) and random arrangement of 48 pieces of catalysts in 6 layers (8 pieces of catalyst in each layer). Because of the random arrangement of these catalysts and development of complex geometry, implementation of suitable computational cells for contact points of catalysts particles was very difficult and time-consuming. In figures (4) and (5) a sample of the developed grids and catalysts arrangements for layers two and three and for two different types of catalysts (No. 3, No. 4) has been shown. Figure (6) showed a schematic of the catalysts arrangement and implemented meshing in some layers for two different shapes of cylindrical catalysts in a bed having a bed-to-catalyst diameter ratio of 4 (N=4).



Figures 4. Arrangement of No. 3 catalyst in N=4 bed

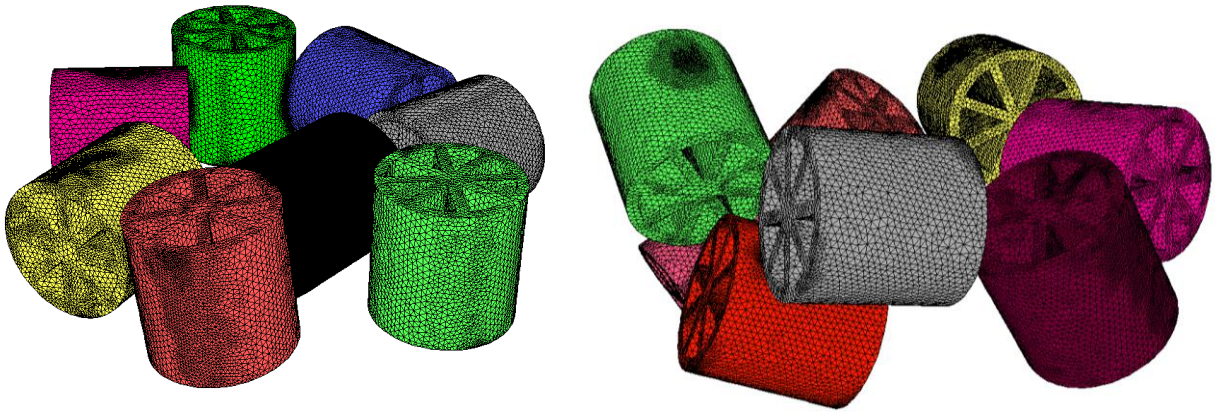


Figure 5. Arrangement of No. 4 catalyst in N=4 bed

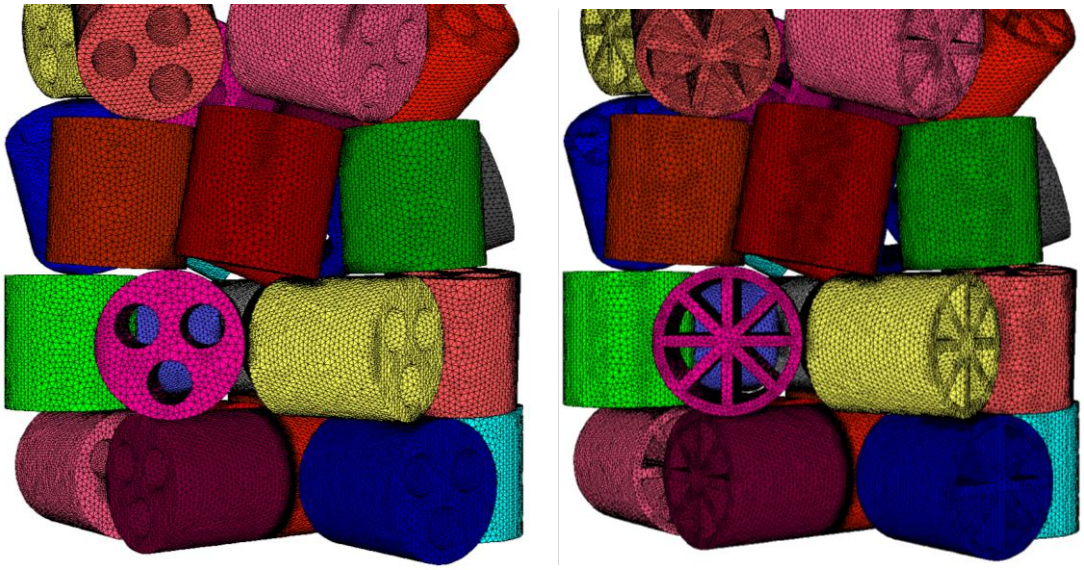


Figure 6. Schematic of catalyst arrangement for 2 catalyst types in N=4 bed

4. Results and discussions

4.1. Validation of the developed computational model

For validation of the developed computational model, experimental data in literature has been used to estimate the heat transfer rate from the walls to the center of the bed. In figure (7) the CFD simulation results have been compared with experimental results [1] adopted from the measurement of the bed temperature radial distributions at two different bed heights. As illustrated in this figure, the results taken from the developed model has got a little deviation from those of the experimental ones. The amount of the error at a bed height of Z = 0.42 m is shown to be 8.52% which is quite acceptable.

4.2. Study of the hydrodynamic parameters and spherical catalysts heat transfer

Figure (8) illustrates the gas flow around the catalyst particles for experimental and industrial conditions with Reynolds numbers of 986 and 25000 respectively. It is shown that there is a complex hydrodynamic around the catalyst particles. It is observed in this figure that the nature of the gas flows for these two Reynolds numbers are diversely different. In high Reynolds number, the separation occurs around the catalyst center while for the low Reynolds number, the phenomenon occurs in last one third of the catalyst. It is also shown in this figure

that the radial mixing of the flows occurs more in low Reynolds number and as the Reynolds number increases, the radial flow mixing decreases.

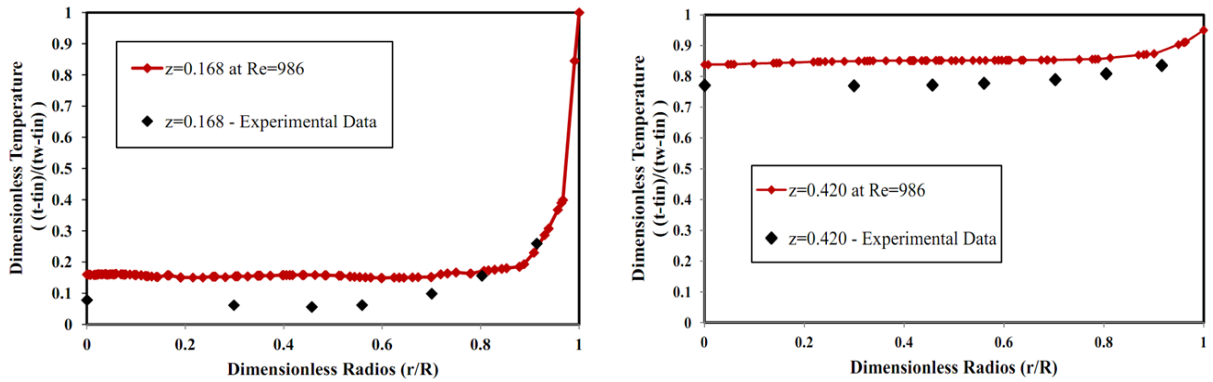


Figure 7. Temperature radial distribution at two different bed heights

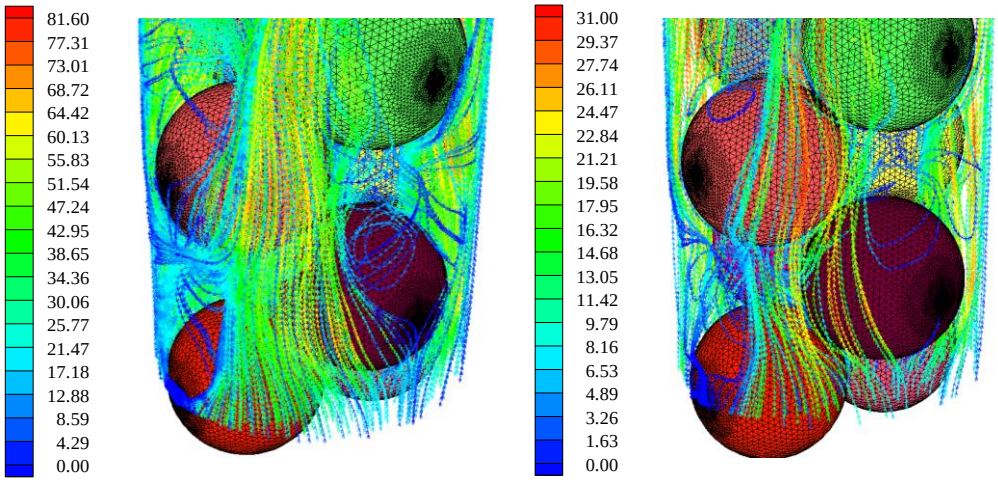


Figure 8. Fluid flow path line around catalysts particles

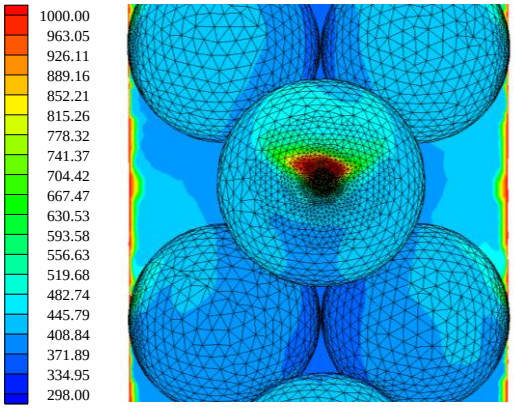


Figure 9. The thermal profile of spherical catalyst particles

Figure (9) demonstrates the thermal profile and the heat transferred from the bed walls to the inner parts of the catalyst particles. It is observed from this figure that the temperature is high near the bed walls and the contact points of the catalysts with the walls but in a little distance from the bed walls, the heat transfer to the bed decrease drastically. According to the thermal profile depicted in figure (9), it is noticed that the temperature penetration from the bed wall to its internal is very low which has a negative impact on reforming reactions and so to increase the efficiency of the reactor, the heat transfer to the bed internal shall get increased.

4.3. CFD simulation of fixed bed reactors with cylindrical catalysts

The main goal of this simulation is to determine the best catalyst geometry and shape that can result in an effective heat transfer and a decrease of pressure drop in beds with bed-to-catalyst diameter ratios of 2 and 4. The governing equations of the gas phase and porous medium have been simultaneously discretized in the form of algebraic equations by applying finite volume numerical method and first and second order upwind discretization scheme. These discretized equations have been solved by means of an upgraded algorithm of SIMPLE [14-15].

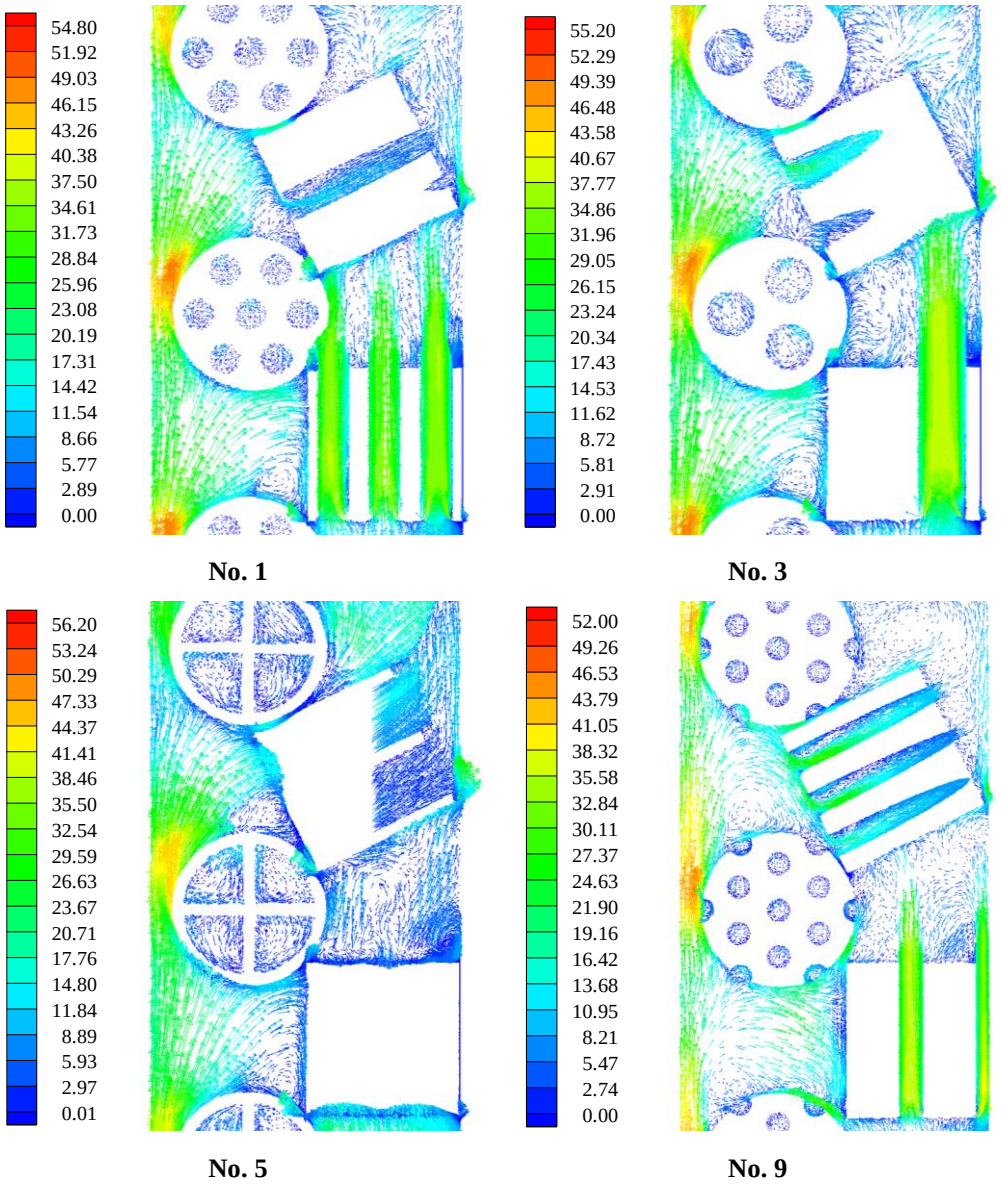


Figure 10. Gas phase velocity vectors around catalyst particles for N=2.

As discussed earlier, there is a complex hydrodynamic around catalysts because of their layout inside the bed and their contact points with the bed walls. Because of this complexity and interaction of the catalysts, the hydrodynamic of the flow and heat transfer is very complex and needs special approaches and optimum computational networks to achieve convergence in CFD simulation. Gas phase velocity vectors around catalyst particles for four different shapes (No. 1, No. 3, No. 5, No. 9) in a specific height of the bed in two cases of bed-to

catalyst ratios of 2 and 4 have been depicted in figures (10) and (11). It is observed from these figures that there is a complex hydrodynamic around catalyst particles which are dependent on their shapes and layout. Also, the results of the CFD simulation show that the maximum gas velocity occurs near the bed walls and the gas near this area gets canalized because of the empty spaces a so leaves the bed without any catalytic reforming reaction. Because of the existence of pseudo plug flows in bed, an optimum layout and shape have to be selected for catalysts to increase radial flows in order to increase the heat transfer and reforming reactions rates and hence improve the efficiency of the synthesis gas conversion.

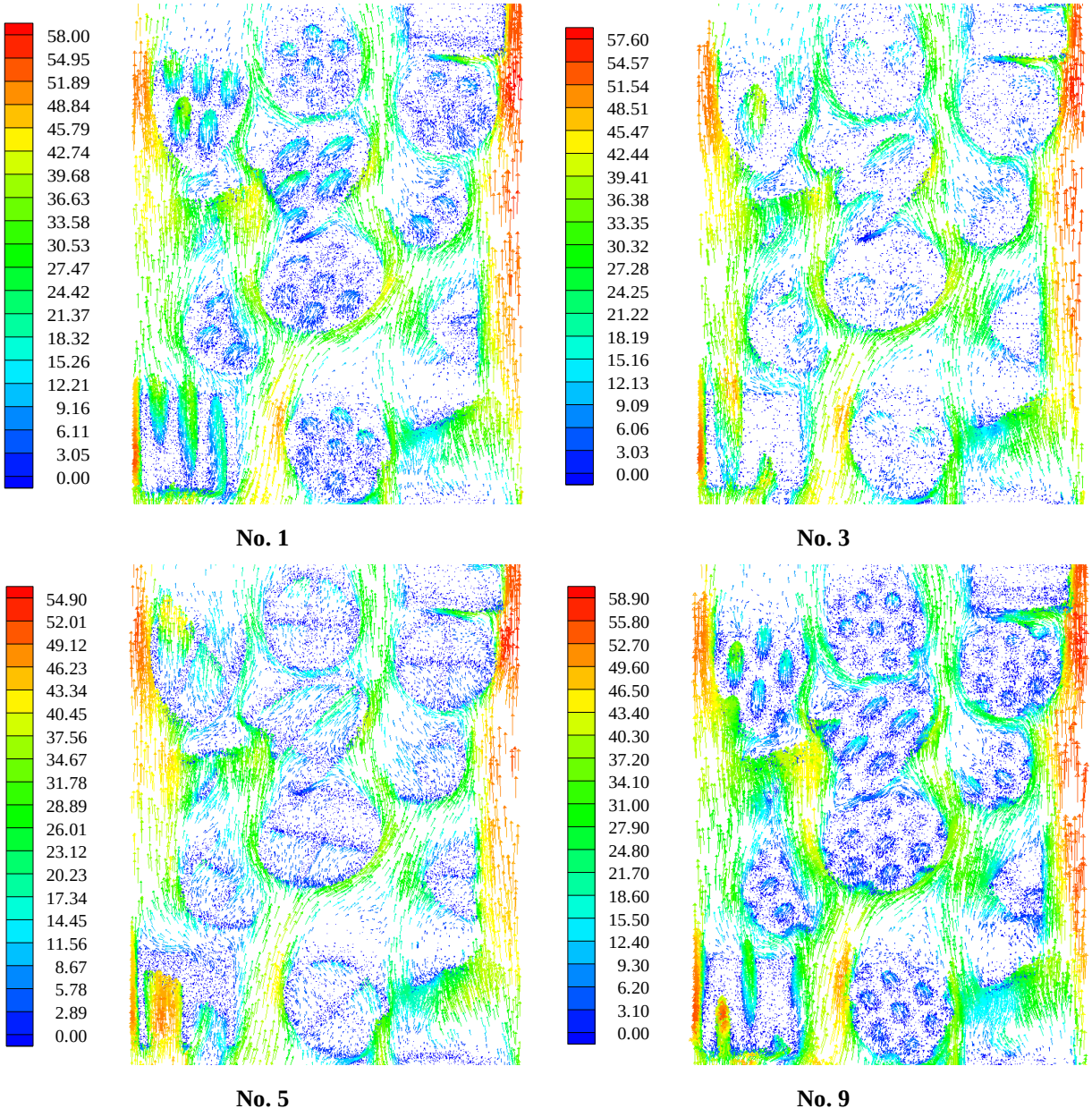


Figure 11. Gas phase velocity vectors around catalyst particles for N=4

The pressure drop amounts for each type of catalyst in bed for N=2 and N=4 at Reynolds number of 12500 and also the mean values of fluid temperatures at bed output have been shown in tables (2) and (3) respectively.

Table 2 Pressure drop and mean fluid temperature at bed outlet for N=2

Catalyst number	Temperature at bed outlet	Pressure drop across bed (Pa)
No. 1	651.4	1285.5
No. 2	660.9	1343.9
No. 3	651.5	1297.6
No. 4	656.1	294.6
No. 5	654.9	292.1
No. 6	659.5	318.71
No. 7	658.2	308.2
No. 8	659.52	300.5
No. 9	656.42	317.5
No. 10	655.4	286.3

Table 3. Pressure drop and mean fluid temperature at bed outlet for N=4

Catalyst number	Temperature at bed outlet	Pressure drop across bed (Pa)
No. 1	628.36	2932.9
No. 2	629.56	3320.1
No. 3	628.66	2871.3
No. 4	627.5	2684.6
No. 5	627.33	2374.9
No. 6	628.83	2999.8
No. 7	629.41	2586.6
No. 8	628.79	2946.1
No. 9	629.55	3068.2
No. 10	626.45	2048.9

It is observed from these tables that the maximum pressure drop and maximum heat transfer to the bed are occurred for catalyst No. (2). It is also noticed from these tables that the rate of pressure drop is coincident with that of the temperature increase of the bed. This happens because in all simulation cases the main reason for pressure drop is the deviation of the fluid from its direct trajectory resulting in radial flows. Radial flows cause an increase of the heat transfer to the bed center. On the other hand, the results given in tables (2) and (3) show that the minimum pressure drop and heat transfer occurs for catalyst No. (10). Also comparing the results of pressure drop and heat transfer rate for two beds (N=2 and 4) reveals that the bed-to-catalyst ratio hasn't got a considerable effect on hydrodynamic and heat transfer characteristics. So it can be deducted that catalyst No. (2) which resulted in the maximum heat transfer can be also suitable for industrial reactors (N=8). Also considering the results taken from CFD simulations and hydrodynamic and heat transfer characteristics, it can be concluded that increase of the catalyst holes and their sizes (an increase of the porosity) has a major impact on system pressure drop and minimum effect on the heat transfer rate to the bed center. It shall be noted that the selection of the best catalyst geometry is dependent on simultaneous simulation of the reforming reactions with flow fields and heat transfer.

5. Conclusion

Although there has been a wide range of researches carried out on steam reforming processes in literature, little studies have been done on catalyst shape and their effects on heat transfer characteristics. In this research, the effects of catalyst shapes on hydrodynamic and heat transfer characteristics were studied using CFD technique. Considering the catalyst particles as porous media, the effect of their thermal conductivity on the heat transfer from the walls to the bed center was investigated. To validate the computational model, experimental data for prediction of heat transfer rate from spherical catalysts to bed centers cited in literature were used. Comparing the results taken from simulation with those of the experimental data on temperature radial profile at different heights of the bed, it was observed that the

mean relative error resulted from the computational model at the height of Z=0.42 m was 8.52%. Regard to the obtained error, it was concluded that the developed computational model could well predict with an acceptable error the hydrodynamic and heat transfer characteristics of a bed with spherical catalysts. In next stage of this study, the validated model was used to investigate the effects of 10 different shape of cylindrical catalysts on hydrodynamic and heat transfer characteristics of a fixed bed reactor with bed-to-catalyst diameter ratios of 2 and 4 (N=2 and 4). The results taken from CFD simulations showed that there is a complex hydrodynamic around catalyst particles because of their layout and the contact points between them and the bed walls. The results showed that the trend of the pressure drop increase was coincident with that of the bed temperature increase and this occurred because the main reason of pressure drop increase was actually deviation of the fluid flow from direct trajectory forming radial flows. On the other hand, the existence of radial flows in bed caused an increase of the heat transferred to the bed center. Comparing the amounts of the heat transfer and pressure drop for two beds of N=2 and 4 showed that increase of the bed-to-catalyst diameter ratio didn't have much impact on the hydrodynamic and heat transfer characteristics. So catalyst No. 2 which had the highest amount of heat transfer to the bed center was concluded to be also suitable for the industrial case (N=8). The results of the CFD simulations as well as hydrodynamic and heat transfer characteristics indicated that increase of the hole numbers as dimensions on the catalyst particles (an increase of the catalyst particles porosity) has a major effect on pressure drop reduction while it plays a minor role in the decrease of the heat transfer to the bed center. Considering the results adopted from the developed model, it was observed that the maximum pressure drop across the bed and the maximum heat transfer to the bed center were obtained from the cylindrical catalyst having a single hole with a small diameter.

Nomenclature

C_{ij}: *Prescribed matrices in porous media*
$C_{1,2,\mu}$: *RNG k- ε constant*
D_{ij}: *Prescribed matrices in porous media*
k: Turbulent kinetic energy
N: bed-to-particle diameter ratio
S: Stress tensor
Re: Reynolds number
T: Thermodynamic temperature
v: Velocity
C_P: *Specific heat*
d_m: *Pore size*
G: Production of turbulent kinetic energy
k_{eff}: *Effective conductivity*
No: Catalyst shape number
P: Pressure:
S_i: *Cumulative momentum*
t: Time

Greek symbols

α: Permeability
σ: Turbulent Prandtl number
μ: Viscosity
ρ: Density
β: Inertial resistance coefficient
ϕ: Void fraction in porous media
Δn: Thickness of porous media in each direction
ε: Turbulent dissipation rate

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To whom correspondence should be addressed: Assistant professor Dr. Yaghoub Behjat, Process Development and Equipment Technology Division, Research Institute of Petroleum Industry (RIPI), Tehran, Iran