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Simulation of the Flow in a Packed-Bed with and without a Static Mixer by Using CFD Technique

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Abstract**—**The major focus of this work was to characterize hydrodynamics in a packed-bed with and without static mixer by using Computational Fluid Dynamic (CFD). The commercial software: COMSOL MULTIPHYSICS^{TM} Version 3.3 was used to simulate flow fields of mixed-gas reactants i.e. CO and H_2. The packed-bed was a single tube with the inside diameter of 0.8 cm and the length of 1.2 cm. The static mixer was inserted inside the tube. The number of twisting elements was 1 with 0.8 cm in diameter and 1.2 cm in length. The packed-bed with and without static mixer were both packed with approximately 700 spherical structures representing catalyst pellets. Incompressible Navier-Stokes equations were used to model the gas flow inside the beds at steady state condition, in which the inlet Reynolds Number (Re) was 2.31. The results revealed that, with the insertion of static mixer, the gas was forced to flow radially inward and outward between the central portion of the tube and the tube wall. This could help improving the overall performance of the packed-bed, which could be utilized for heterogeneous catalytic reaction such as reforming and Fischer-Tropsch reactions.

Keywords**—**Packed Bed, Static Mixer, Computational Fluid Dynamic (CFD).

I. Introduction

IN a fix-bed reactor design, flow pattern, heat transfer, and mass transfer have usually been studied by using a small reactor or lab-scale reactor before the process of scaling-up is conducted. The problem of understanding and predicting of fluid flow in a fixed-bed reactor is one of long-standing. A recent new approach to this problem is the use of computational fluid dynamics (CFD) to model fluid flow patterns, and thus to contribute to improving our understanding of the system. This results in an achievement of an optimal and safe design of this type of reactors.

The catalyst particle designs for fixed bed reactors are governed by several considerations, such as pressure drop of the bed, catalyst effectiveness for reaction, particle crush strength, and heat transfer efficiency. For example of methane steam reforming, the gas flow rate is very high, that forces the use of large catalyst particles to reduce pressure drop, and the reactions are highly endothermic, which requires the small tubes so that heat may be supplied efficiently through the tube wall. The fixed bed reactor tubes have low tube-to-particle diameter ratio (*N*), often in the range of 4–8. Due to the strong diffusional limitations, reaction takes place in a thin layer near the particle surface [1] so that the particles behave like "egg-shell" catalysts, and activity is observed to be proportional to external geometric surface area [2].

Improving steam reforming reactor performance, modern catalyst pellet design has evolved from simple cylinders and rings to include pellet shapes with internal holes and external features, such as lobes and grooves [3]. Larger external surface area for reactant access into the pellets leads to higher catalyst activity, and lower tube wall temperatures and thus longer tube life [2], [4]. Lower pressure drop, or higher plant rates at the same pressure drop, can be obtained, as well as lower methane slip and closer approaches to equilibrium [2]. For improving flow pattern in the reactor, static mixer is used as an advanced device promotes mixing by successively dividing, rotating and redirecting the gas while keeping pressure drops low (reduced compressor power for high flow rates and/or viscous fluids) [5] and the enhancement of radial mass transfer. This reactor may be a new tool for reaction engineers, e.g., to suppress hot-spot formation or for heterogeneously catalyzed viscous liquid-phase reactions [6].

Simulations of steam reformer tubes usually show the complex pellet shapes by equivalent 1-D shapes such as annular rings [1]. Considerable efforts are being made to improve the computation of effectiveness factors by defining shape factors for complex 3-D pellet shapes such as multi-hole and multi-lobe cylinders [7] and "wagon-wheel" type tablets [8]. These shape factors may then be used in 1-D models to approximate the reaction behavior of 2-D or 3-D pellets.

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This studied was focused on the fix-bed reactor for Fischer-Tropsch reaction with and without static mixer by using computational fluid dynamic technique on the 3-D model. Spherical catalysts were modeled in the reactor at the same amount. Flow patterns of fluid distribution in the packed-beds were investigated.

II. Simulation Model and Methodology

The dimensions appeared in the flow simulation of the packed-bed with and without a static mixer were assigned in complying with those used in-progress experiments conducted by the same authors i.e., a single element of the static mixer was 0.8 cm in diameter and 1.2 cm long with the thickness of the metal sheet of 0.1 cm. The detailed geometry of the mixing element in Fig. 1 was summarized in Table I.

TABLE I
Geometry of the Mixing Element (s)

Diameter (cm)	0.8
Length (cm)	1.2
Blade thickness (cm)	0.1
Twisting Angle (per element)(degree)	180

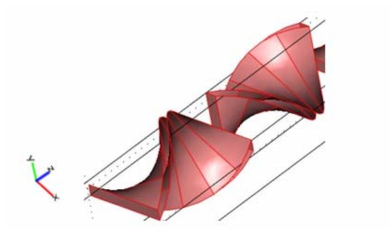


Fig. 1 Geometry of the mixing element (2 elements shown)

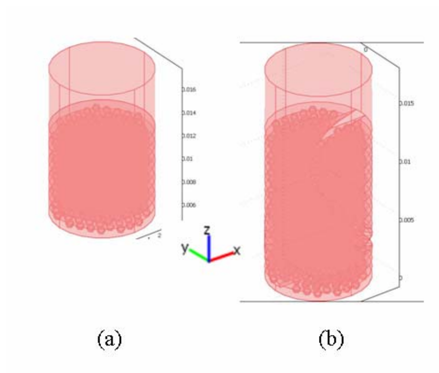


Fig. 2 Computational domain of (a) the conventional packed bed, (b) the packed bed equipped with the static mixer

In the packed-beds with and without a static mixer, approximately 700 spherical particles with a height and a diameter of 650 µm (same shape and size as catalyst pellets used in the experiments) were close packed. The packing applied in the simulation and shown in Fig. 2 was an only one realization among all possible.

The resultant flow fields in the packed beds were obtained by using COMSOL MULTIPHYSICS version 3.3. The characteristics of fluid flow were investigated via the hydrodynamics parameters. The computation of flow was achieved by the mathematical models based upon the conservation principles, namely, the conservation of momentum and mass. In order to obtain the three dimensional flow field, the incompressible Navier-Stokes Equations were utilized i.e.,

$$\rho\frac{\partial u}{\partial t} - \nabla\cdot\eta(\nabla u + (\nabla u)^T) + \rho(u\cdot\nabla)u + \nabla p = 0$$
$$\nabla\cdot u = 0 \qquad (1)$$

where η denotes the dynamic viscosity, u the velocity vector, ρ the density of the fluid, and p is the pressure.

In subdomain setting, the mixed gas (comprising of CO, H_2 at 180 °C) with the effective density of 0.4329 kg/m^3 and viscosity of 1.5x10^{-5} kg/m·s were used in the simulation. The velocity boundary conditions were set such that the velocity of feed gas in the x-direction and y-direction were zero, and the average flow velocity in the z-direction was set in accord with the operational flow rate i.e.,

$$u_{av} = \frac{\dot{Q}}{A} \qquad (2)$$

where u_{av} is the average velocity, Q is the volumetric flow rate, A is the cross-sectional area of the tube. Thus, the inlet flow was set as a parabolic velocity profile, and the exit flow was set as neutral i.e., the normal component of the viscous term of the Navier-Stokes Equations was set as null as stated in Equation (3).

$$\eta(\nabla u + (\nabla u)^T)n = 0 \qquad (3)$$

Others boundary conditions were set as no-slip. Typical mesh size used was set as fine with 168450 and 241471 finite elements for the case of the packed-bed with and without the static mixer, respectively as seen in Fig. 3.

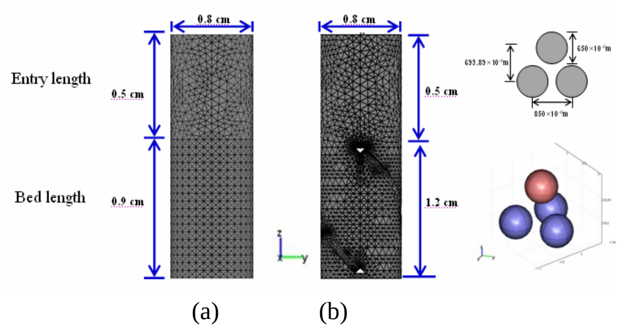


Fig. 3 Mesh size and catalyst structure for (a) the conventional packed bed (b) the packed bed equipped with the static mixer

For comparison and design purposes, velocity flow profiles were determined for the conventional packed-bed and the static mixer type packed-bed both at an inlet volumetric flow rate of 30 ml/min.

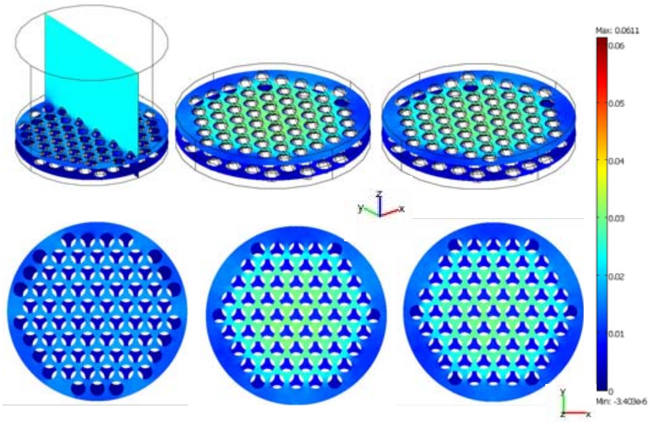
III. Simulation Results and Discussion

The computational domain adopted in the simulation was shown with dimensions in Fig. 2. The mixer diameter is 0.8 cm, and thus minimizes the air slip at the reactor wall. Usually in an application, there is a certain distance of flow within a pipe so that the gas flow can develop into the fully developed condition before entering into the packed-bed. Thus, the incoming flow was properly assumed to be fully developed. In the range of gas flow velocity encountered in the reactions, the flow can suitably be considered as incompressible. In this study, the hydrodynamics of the gas flow within the packed bed reactor incorporated with a static mixer was investigated in parallel with the case of the conventional packed bed. The heights of each bed were set slightly differently due to the space required for catalyst packing; however, the mass of catalyst were the same and the comparison was considered based on the same gram of catalyst.

Figs. 4 and 5 illustrated the pressure fields of the conventional and the modified with static mixer packed beds. The resultant pressure drops were 0.008947 Pa for the former, and 0.000388 Pa for the latter per double layers of packed catalyst. The pressure drop of the modified bed was lower comparing with that of the conventional bed. This is probably caused by the computational setup of the solid catalysts within the bed that causes more void in case of the static-mixer-modified bed. Nevertheless, these figures were subjected to a certain level of indeterministic of the packing configurations which in turn affects the flow-solid interaction. The pressure drop inferred from the simulation in the case of the conventional packed bed was close to the value estimated from Blake-Kozeny empirical equation for the laminar flow regime.

$$\Delta P = 150 \cdot L \cdot \frac{(\mu \cdot u)}{d_p^2} \cdot \frac{(1-\varepsilon)^2}{\varepsilon^3} \tag{4}$$

where ΔP is the pressure drop, L is the column length, d_p is the mean particle size, ε is the porosity and $(1-\varepsilon)$ is the void fraction.



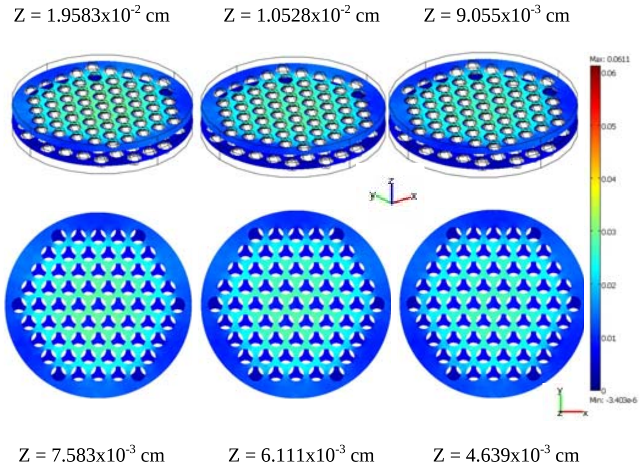


Fig. 4 Pressure distribution within the conventional packed bed

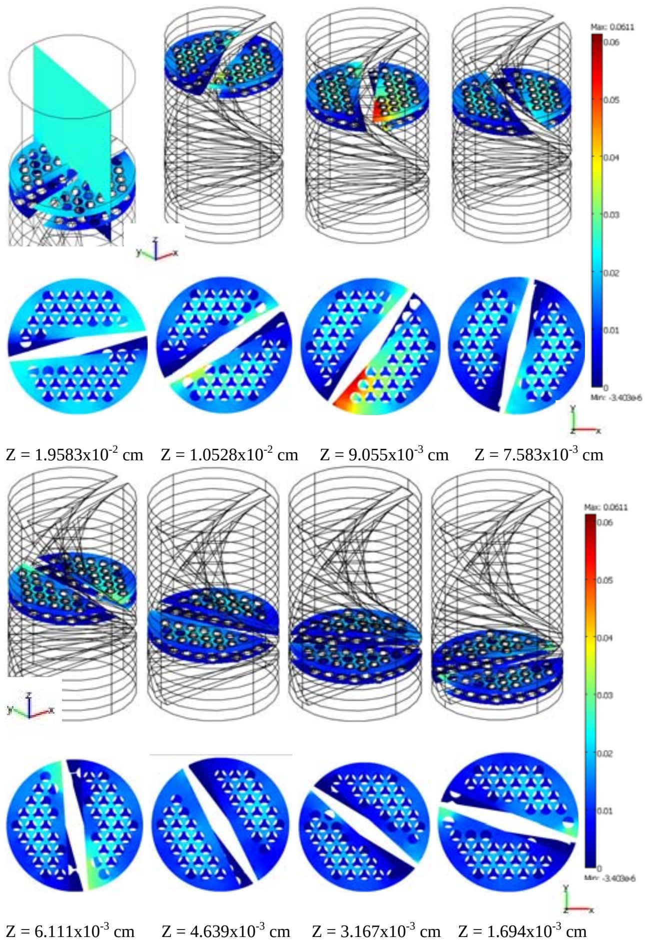


Fig. 5 Pressure distribution within the packed bed equipped with the static mixer

In addition to the pressure variation in the axial flow direction, the pressure field of modified bed also exhibited the strong variation along the radial and circumferential directions. These pressure gradients played a role in gas distribution, which in turn affected the momentum transfer. The corresponding heat and mass transfers in the case of reaction flow were expected to be enhanced in such case.

From Fig. 6, the total velocity plot showed that the fluid flew around the catalyst pellets and a confined channel. The gas flow was accelerated as it passed into the gaps between the pellets as obviously seen in Fig. 6. The main flow in the axial direction was enforced, and the average flow rate determined at each axial location was made rather uniform. Since the simulation was conducted at the design flow for the FT reactor application, therefore the corresponding value of Reynolds number was set at 2.31. At this range of Re, the small scale swirling flow i.e., local eddies were observable clearly especially between the adjacent catalyst pellets. Due to the shape of the pellet, the vortices tended to emanate from the sharp edge of the pellets where the flow separation occurred. In Fig. 7, the gas flow was directed to flow inward and outward in the radial direction by the presence of the static mixer.

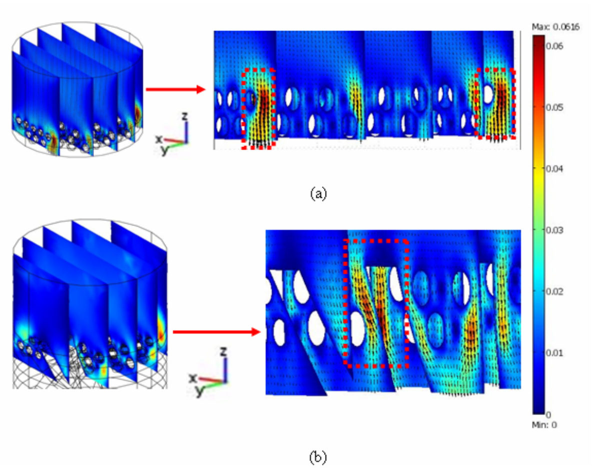


Fig. 6 The total velocity and arrow velocity (a) the conventional packed bed, (b) the packed bed equipped with the static mixer

The static mixer induced the out-of-plane velocity components as obviously seen in the slices of vector presentations in Fig. 7b. The high velocity gradients especially in the radial and circumferential directions were expected to promote the transport phenomena between the solid catalyst and the gas phase reactant due to the enhanced local transport parameters.

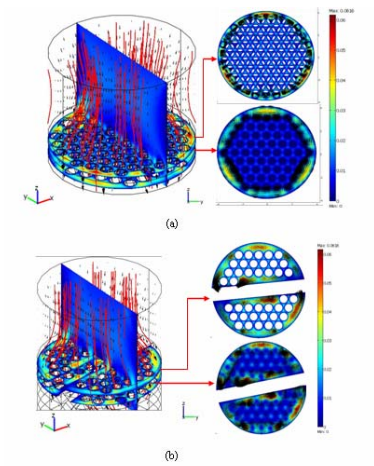


Fig. 7 Streamlines, total velocity and cross sectional plot of the total velocity at selected cross sections (a) the conventional packed bed, (b) the packed bed equipped with the static mixer

For general comparison, Fig. 7 showed the flow patterns of both the conventional and modified packed bed at a cross section that had approximately the same area ratio of the catalyst phase to the gas phase. At this axial location, the packed bed with the static mixer showed a well-defined pair of peak velocity on the opposite sides of the static mixer, and almost stagnant zones located off diagonal of the static mixer as shown in Fig. 7b. A large portion of high velocity and velocity gradient were in contact with the catalyst surface in the case of modified bed. On the other hand, from Fig. 7b, comparatively smaller portion of catalyst could effectively react to the gas flow due to low flow magnitude. The flow pattern was also rather distributed randomly in the conventional bed comparing with the pattern emerged in the static mixer type bed as further shown in Fig. 8 and 9. Fig. 8 and 9 illustrated the evolution of velocity field at different axial planes that were equally spaced from the top to the bottom planes of each bed.

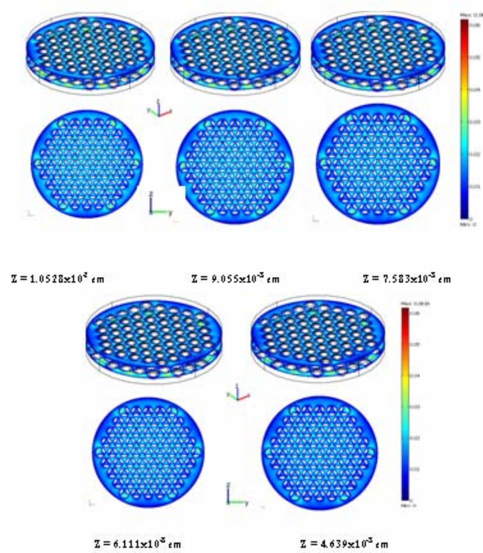


Fig. 8 Variation of velocity contour in the axial cross sections within the conventional packed bed

From Fig. 8, the interaction between the catalyst and gas flow could be low because of the improper distribution causing ineffective contact between the two phases. On the contrary, for the static-mixer type reactor, well-defined distribution pattern existed on every cross section as illustrated in Fig. 9, and the uniformity of transport phenomena occurred in the modified bed was apparent. The reason is that the static mixer divided the flow area into separated smaller zones, and the reactant gas is directed to flow inward and outward in the radial direction with strong centrifugal effect. The induced symmetric or skew-symmetric velocity distributions were in accord with the twisting pattern of the static mixer but in both case the catalyst pellets well interacted with the gas flow. The magnitude of the flow velocity was always higher because of the smaller flow area and this implied better transport characteristics.

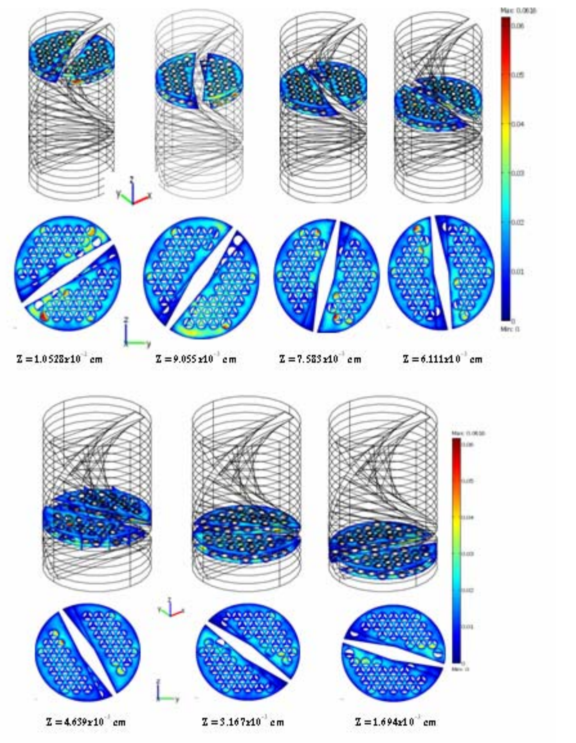


Fig. 9 Variation of velocity contour in the axial cross section within packed bed equipped with the static mixer

IV. Conclusion

The following conclusions were drawn from the simulation results of this study; however, the results were based on only one realization of the packing. The model consisted solely of a detailed hydrodynamics platform. The packed-bed modified with the static mixer decreased the GSV as twice as large compared with that of the conventional bed, and thus increased the effectiveness of reaction surface area between the solid catalyst and the gas flow by directing the flow in the radially inward and outward direction to pass the individual particles representing catalyst pellets. The static mixer induced the higher local velocity gradient in the flow field. The rate of momentum transfer was readily be ensured from the simulation, and the heat and species transfers could also be strongly expected to be effectively enhanced as well.

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