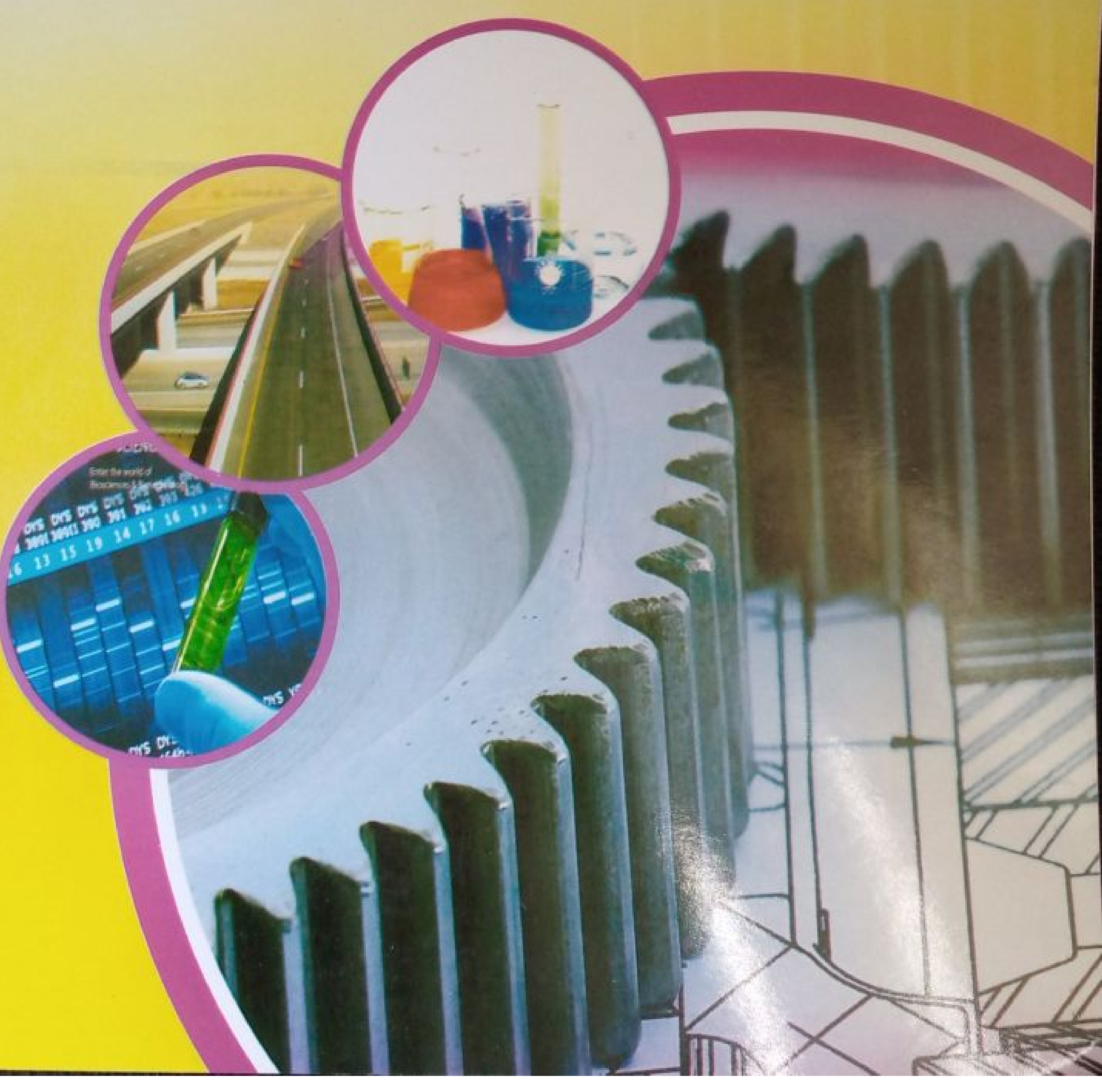
FEDERAL UNIVERSITY OF TECHNOLOGY
MINNA
Technology for Empowerment

NIGERIA JOURNAL OF ENGINEERING AND APPLIED SCIENCES (NJEAS)

Volume 5, No. 1 - 2018
ISSN: 2465 - 7425



NIGERIA JOURNAL OF ENGINEERING AND APPLIED SCIENCES (NJEAS)

Nigeria Journal of Engineering and Applied Sciences - NJEAS (ISSN:2465-7425) is a peer reviewed research journal jointly published by School of Infrastructure, Process Engineering and Technology and School of Electrical Engineering Technology, Federal University of Technology, Minna, Nigeria. The journal covers all engineering and science disciplines and aims to publish high quality theoretical and applied papers that will be important contributions to the literature. We welcome submissions in the journal's standard format in MS-Word file through our email.

PUBLISHED BY:
School of Infrastructure, Process Engineering and Technology and School of Electrical Engineering Technology,
Federal University of Technology, Minna – Nigeria.

ALL CORRESPONDENCES TO:
Editor - in – Chief
Nigeria Journal of Engineering and Applied Sciences (NJEAS)
School of Engineering and Engineering Technology,
Federal University of Technology, P.M.B 65, Minna – Nigeria
E-mail: njeas@futminna.edu.ng, Website: njeas.futminna.edu.ng

CONTENTS

Nigeria Journal of Engineering and Applied Sciences (NJEAS) Vol. 5, No. 1, 2018

CFD Analysis of Pressure Drop of Hydrogen Gas Flow in a Packed Bed

Afolabi, E. A. and Andeyabin, S.

Chemical Engineering Department, Federal University of Technology, Minna, Nigeria
E-mail: elizamos2001@yahoo.com

Abstract

The understanding of pressure drop prediction through packed beds of adsorbent is vital as pressure drop determines the operating cost and cost of energy consumption. Computational fluid dynamics (CFD) simulation was performed using ANSYS Fluent 14.0 CFD package to study the effects of different parameters such as particle size, bed porosity and fluid velocity on pressure drop. This study employed a single phase flow in a porous media of packed bed with hydrogen gas and activated charcoal as the fluid and adsorbent respectively. The CFD results were validated against theoretical data obtained from Ergun's pressure drop equation. CFD results show good agreement when compared with the theoretical data. Finally, a parametric study demonstrated the effect of particle size and porosity to be inversely proportional, while fluid velocity was observed to have a direct effect on the pressure drop of hydrogen gas flow in a packed bed.

Keywords: Adsorbent, Computational Fluid Dynamics, Packed beds, Pressure drop, Porosity, Simulation

---

Introduction

Packed beds have gained a global recognition over the years for their versatile application in chemical industries such as solid extraction, distillation, catalytic heterogeneous reaction, adsorption, absorption/desorption of gases (Zabelata, 2007). The application of packed beds in engineering and industrial processes varies and this variation might involve packed bed reactors in nuclear plants, catalytic reactors, and thermal storage used in replaceable and sustainable energy systems (Theron, 2011). It plays a significant role by ensuring that the contact between the phases within the bed is improved and the basic principle in all packed beds remains the same irrespective of their applications (Theron, 2011). Pressure drop over packed beds is the most important parameter that must be accurately predicted when designing any system that incorporates packed bed, pressure drop determines the pumping power and operating cost in a packed bed system (Kruger *et al.;* 2015). The essential motivation in studying packed beds is to regulate the significant operating cost of the pressure drop through the packed adsorbent bed (White, 2016).

The application of CFD as a standard tool for fluid flow, heat and mass transfer analysis and associated phenomena is on the increase due to advancement in computing technology. This increase has been motivated by progressive computer speed, systems affordability and accessibility to new commercial CFD software thereby resulting into higher preference for CFD simulation in comparison to prototype experiments (White, 2012). The packing and arrangement of the small particles in a fixed container easily facilitate close contact between fluids of various combinations used in different processes (Catalysis, ion exchange, sand filtration, absorption, distillation, and adsorption and heat storage) in chemical plants (Baker, 2011). Packed bed is the subject of this study and focuses on the resistance caused by the presence of particles obstructing fluid flow within the bed. This makes the understanding of pressure drop prediction through packed bed of adsorbent an important area of research as pressure drop determines the operating cost and cost of energy consumption. For example, an efficient operation of packed towers requires low pressure drop as well as energy of consumption. In a filtration system, pressure drop is an important factor to be considered due to fluid that flows through the filter medium by virtue of a pressure differential across the bed (Geankoplis, 2003). Investigating the pressure drop across the bed is therefore crucial to determine filtration efficiency and expected time span before excessive buildup of filtered material occurs.

Niaei *et al.* (2009) suggested that simulation of chemical process has been proven as the most reliable and safest way to investigate and predict the effects of influencing parameters on a flow process. This involves the application of the concept of computational fluid dynamics as a theoretical approach to investigate and predict the performance of a process that involves fluid, heat and mass transfer. Mohammadikah *et al.* (2014) reported the improvement of hydrodynamics performance of Naphta catalytic reforming reactions using CFD. The simulation results of their study showed that, small velocity result into small pressure drop and greater velocity lead to an increase in pressure drop across the bed. They concluded that there is a linear relationship between velocity and pressure drop across the bed. In addition, higher pressure drop was observed in turbulent case regime in comparison with the laminar regime. The aim of this work is to study the CFD simulation of hydrogen gas flow through a packed bed filled with activated charcoal (adsorbent) using ANSYS Fluent 14.0 package. To achieve this, pressure drop across the porous medium in the packed bed was numerically simulated and results were compared with theoretical data obtained from Ergun equation. The parametric study of the effect of different parameters (particle size, porosity of the bed, fluid velocity and bed height) on pressure drop of hydrogen gas flow across a activated charcoal packed bed were investigated and optimum level determined

Numerical Methodology

Computational Domain

The geometry used in this work was created using ANSYS FLUENT 14.0 design modeller to create a three-dimensional model of a packed bed in form of a vertical cylindrical pipe with a dimension of 50 *mm* height and 5 *mm* diameter. As shown in Fig. 1, the whole geometry is made up of three sections with the middle section set as the porous zone and filled with activated charcoal as adsorbent material. This geometry corresponds to a 3D numerical solution domain with dimension of 50 mm, 50 mm and 5 mm in radial, axial and tangential direction respectively.

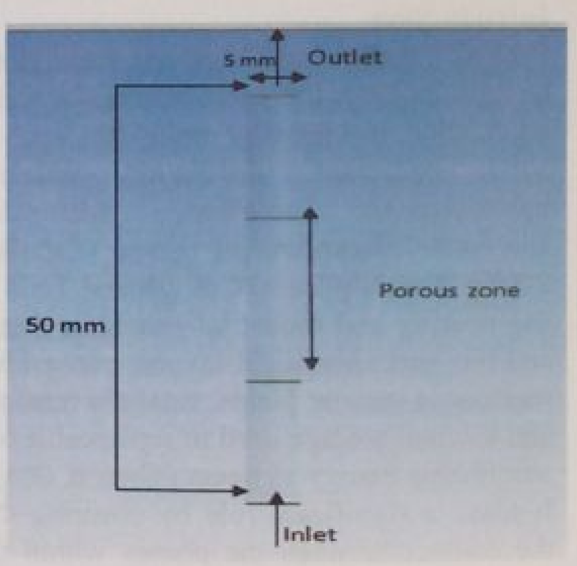
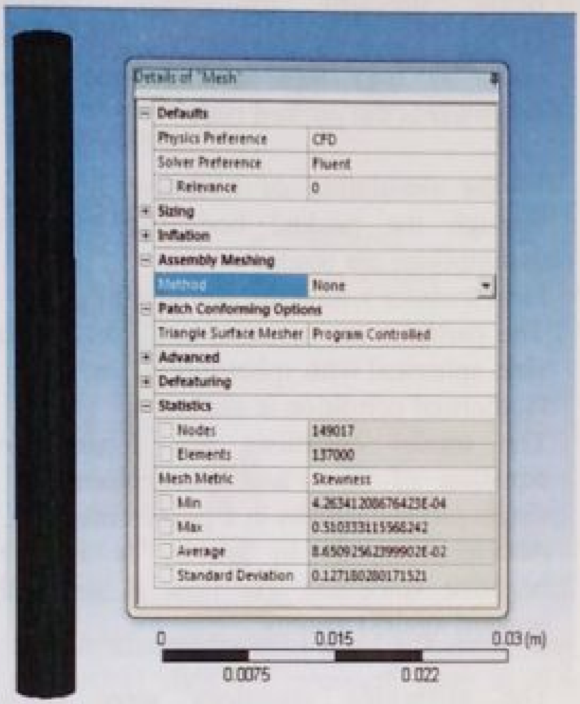


Fig.1: Geometry of the CFD Domain

Mesh Generation

Meshing of the geometry was carried out using ANSYS ICEM CFD to discretize the fluid domain with Multizone method used for meshing and total thickness selected for the inflation option. The relevance centre, curvature and smoothing options were set to fine, off and high respectively in order to archive maximum accuracy. Walls are chosen as stationary with a no slip condition, meaning that the velocity in the flow- and the normal direction of the walls are equal to zero (Versteeg and Malalasekera, 2007). The inlet of the bed was defined as velocity inlet with the velocity being specified based on the hydrogen gas flow rate. The outlet of the bed was defined as pressure outlet at the packed bed pressure. Fig. 2 gives detail of the mesh geometry used to perform the CFD simulations.



Details of "Mesh"

Defaults	
Physics Preference	CFD
Solver Preference	Fluent
Relevance	0
Sizing	
Inflation	
Assembly Meshing	
Method	None
Patch Conforming Options	
Triangle Surface Mesher	Program Controlled
Advanced	
Defeaturing	
Statistics	
Nodes	149017
Elements	137000
Mesh Metric	Skewness
Min	4.26341200676423E-04
Max	0.510333115568242
Average	8.65092562399902E-02
Standard Deviation	0.127180280171521

Fig 2: Details of the mesh geometry

Grid Independence Test

Grid independence analysis was carried out with a steady state computation of three different grid cells of 44756, 64800 and 137000 with orthogonal quality of 0.826652, 0.8393343 and 0.806552 respectively. This test was aimed at checking the influence of the size of the grid on the numerical simulation result. The same numerical simulations were performed for the three different grid sizes with hydrogen flowing at 0.1 m/s velocity, 250 μm particle diameters and 0.6 porosity. The results of the pressure drop in a plane of interest were examined and the grid cell of 137000 found to be fine enough for an accurate simulation as the increase in grid size was observed to have negligible effect on the pressure drop. Hence, a grid size of 137000 was then used for the numerical simulation of hydrogen gas flowing through activated charcoal in a packed bed.

Governing Equations

Flow through porous media is modeled by adding an extra source term to the standard flow equations by using the Forchheimer equation (Equation 5). Equations 6 and 7 show how the source term is defined in ANSYS FLUENT for the case of simple homogeneous porous media (ANSYS Fluent, 2011). The conservation equations of mass and momentum are solved iteratively until convergence is observed at steady state. The mass and conservation equation of a single phase in a porous media includes:

Continuity equation

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

Equation (1) is the general form of the mass conservation equation and is valid for both compressible and incompressible flows. ρ is the density of the fluid and $\vec{v}$ is the velocity vector of the fluid and t is the time.

Momentum conservation equation

$$\frac{\partial(\rho\vec{v}\vec{v})}{\partial t} + \nabla.(\rho\vec{v}) = -\nabla P + \nabla.\tau + \rho\vec{g} + \vec{F} \quad (2)$$

In the equation 2, P is the static pressure, τ is the stress tensor, $\vec{g}$ is the acceleration due to gravity, and $\vec{F}$ represents all external body forces of the system which also contains other model dependence source terms such as porous-media and user-defined sources (Qasim *et al.*, 2011, Pandey, 2011). The stress tensor is given as:

$$\tau = -\mu[(\nabla\vec{v} + \nabla\vec{v}^T)] - \frac{2}{3}\mu\nabla.\vec{v}I \qquad (3)$$

where μ is the molecular viscosity and τ is the unit tensor and the second term on the right hand side represents the effect of volume dilation.

The Ergun equation

Ergun Equation provides a correlation in term of viscous and kinetic losses for the pressure drop of a fluid flowing through a bed packed with uniform size particle (Mousazadeh, 2013). For spherical particles with uniform particle size, the Ergun equation of pressure is given as:

$$\frac{\Delta P}{L} = \frac{150\mu}{d_P^2\phi_P^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}v + \frac{1.75\rho}{d_P\phi_P}\frac{(1-\varepsilon)}{\varepsilon^3}v^2 \qquad (4)$$

where ϕ_P is the particle sphericity (which is one for spherical particles). Alternatively, equation 4 can be written in a simpler form as:

$$\frac{\Delta P}{L} = \frac{\mu}{\alpha}V + \frac{1}{2}C\rho V^2 \qquad (5)$$

where permeability and inertia loss coefficient may be determined theoretically as:

$$C = \frac{3.5}{\Delta P}\frac{(1-\varepsilon)}{\varepsilon^3} \qquad (6)$$

$$\alpha = \frac{d_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2} \qquad (7)$$

Numerical Simulation of hydrogen flow in a packed bed

A segregated, 3-D double precision implicit solver of ANSYS Fluent was activated and the 3D grid from ANSYS ICEM CFD meshing scheme imported into ANSYS Fluent solver for the simulation of hydrogen gas flow in a 5 mm ID packed bed. Pressure based solver is selected for the CFD simulations and the conservation equations of mass and momentum are solved iteratively by converting a set of non-linear equations coupled to one another in which the set of the equation are solved repeatedly until the solution converged. Energy conservation equation is neglected because there is no heat transfer within the system. The domain is divided into discrete control volume using a computational grid in which integration of the governing equations on the respective control volume take place by constructing algebraic equations for the discrete dependent variables followed by linearization of the discretized equations to obtain updated values of the dependent variable (ANSYS Fluent, 2011). The enhanced wall function was used for the near-wall treatments of the wall boundaries. Operating conditions were specified as being standard atmospheric pressure (101325 Pa) with gravitational acceleration taken as 9.81 m/s^2 and defined to act downwards the packed bed.

In the simulation of hydrogen gas flow through the packed bed, the following assumptions are made:

- ✓ Heat transfer within the bed is negligible.
- ✓ The particles are assumed to have uniform size, spherical with sphericity of one.
- ✓ Isothermal condition is assumed.
- ✓ The model equations are conservation equation of mass and momentum for a single phase gas flow in a porous media.
- ✓ Acceleration due to gravity is assumed negative since the gas flow is vertically upward against gravity.

The governing equations were solved applying an implicit finite volume technique embedded in ANSYS Fluent. For pressure velocity coupling, the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm was used. The convective terms in all governing equations were initially discretized by means of a first Order-Upwind scheme, then after higher schemes activated and simulation continue until convergence was established. The porous media model was used to solve the gas flow distribution through the packed bed. The viscous loss coefficient ($1/\alpha$) and the inertial loss coefficient (C_2) values were calculated based on the material properties of the activated charcoal and the gas flow as specified in Equations 6 and 7.

Results and Discussion

The CFD simulation of hydrogen gas flow in a porous packed bed was carried out using ANSYS Fluent 14.0 software and results presented in term of the pressure drop along the bed. The effectiveness of the CFD models in predicting the pressure drop of hydrogen flow in a packed bed was then determined by comparing the simulated with the theoretical data obtained from simplified form of Ergun pressure drop equation. The effect of the various parameters on the pressure drop of hydrogen gas using the CFD models was also studied.

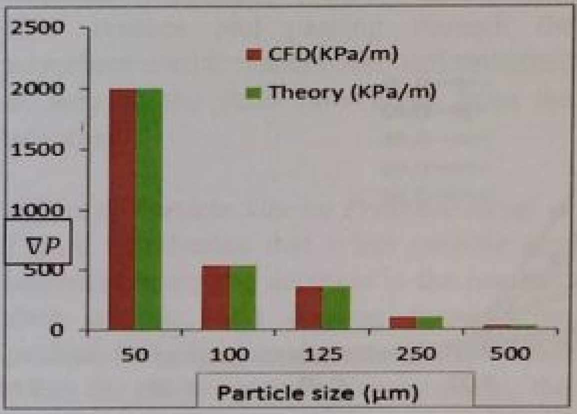


Fig. 3: Comparison of the CFD result and theoretical data for pressure drop at 0.6 porosity, 5 m/s fluid velocity and different particle sizes.

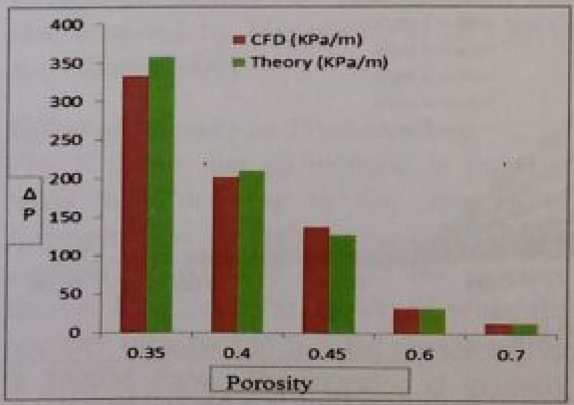


Fig. 4: Comparison of the CFD result and theoretical data for pressure drop at 500 µm particle size, 5 m/s fluid velocity and different porosities.

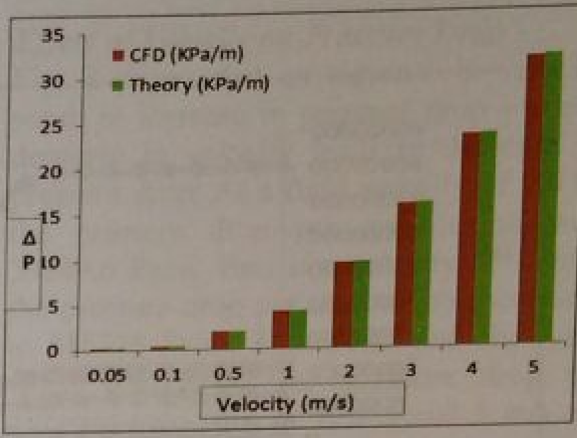


Fig. 5: Comparison of the CFD result and theoretical data for pressure drop at 500 µm particle size, 0.6 porosity and different fluid velocities

Validation of CFD Simulations

In validating the simulation results, the CFD results obtained were compared with theoretical data obtained from simplified form of Ergun pressure drop equation. Figs. 3 to 5 showed the comparison between the theoretical data and the predicted results obtained through CFD analyses. The pressure drop profile as shown in Fig. 4 is observed to be over-predicted in the CFD simulation at 50, 100 and 500 µm and under-predicted at 125 and 250 µm particle sizes. For example, the predicted pressure drop of hydrogen flow through packed bed at particle size of 50 µm is 2000 KPa/m, while the theoretical result is 1999 KPa/m. The maximum and minimum difference when comparing the CFD predicted pressure drop with the theoretical data are 0.888 % and 0.026 % at 250 µm and 125 µm particle size respectively. The same trend in term of agreement was exhibited by the CFD predicted and theoretical pressure drop profiles at different velocity and porosity as shown in Figs. 3 and 5 respectively. This shows a good agreement between CFD pressure drop and theoretical pressure drop using Ergun equation.

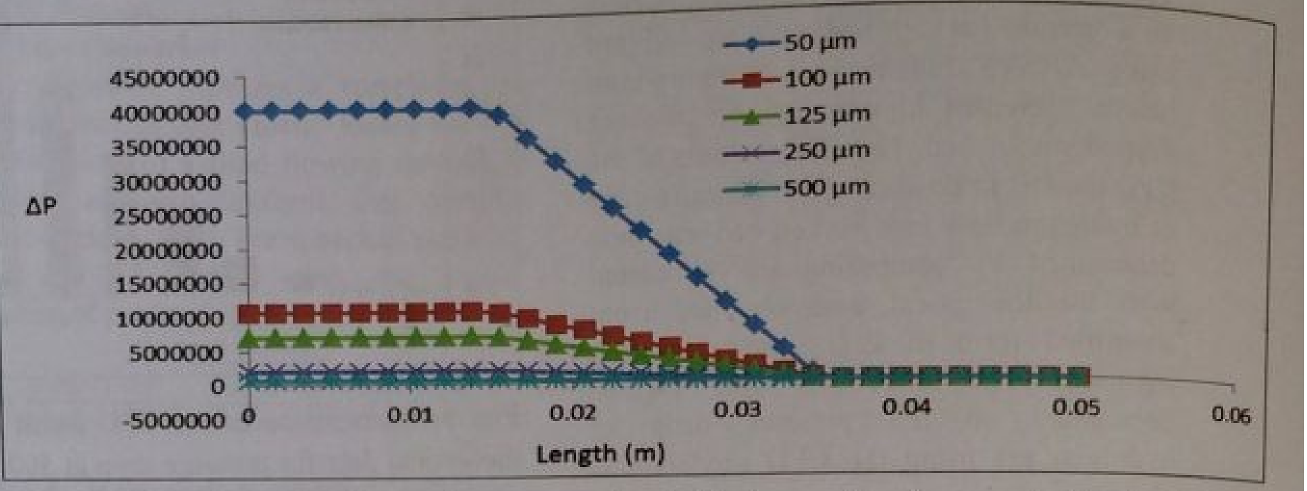


Fig. 6: Effect of particle size on the pressure drop of hydrogen flow in a packed bed at 0.6 porosity and fluid flow velocity of 5 m/s.

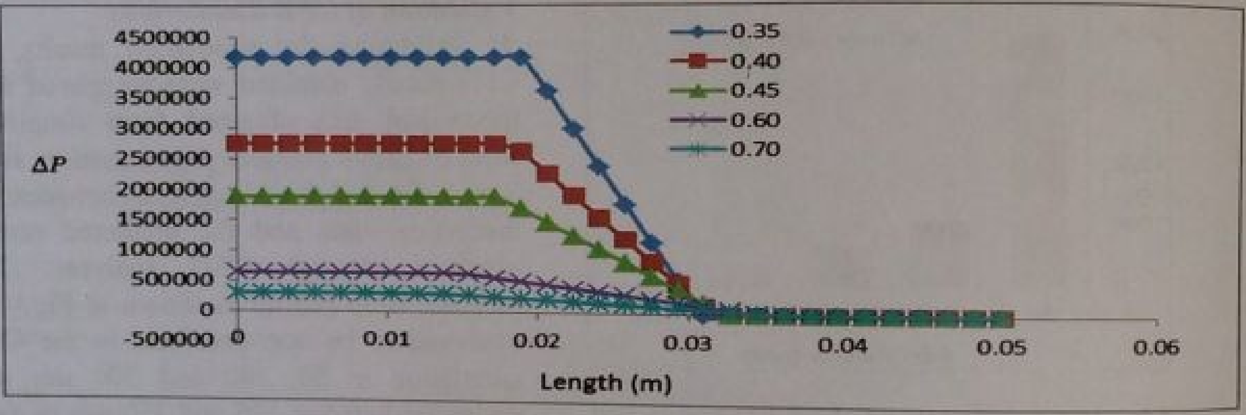


Fig. 7: Effect of porosity on the pressure drop of hydrogen flow in a packed bed at 500 µm particle size and fluid velocity of 5 m/s.

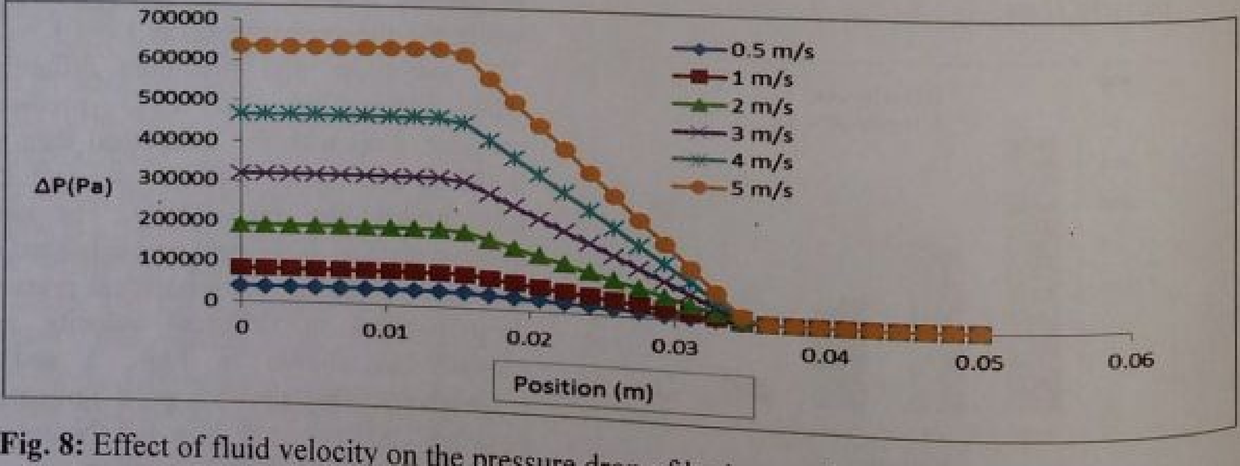


Fig. 8: Effect of fluid velocity on the pressure drop of hydrogen flow in a packed bed at 0.6 porosity and 500 µm particle size.

Investigating the Effects of Process Variables

The validity of numerical simulation of the pressure drop predicted for hydrogen gas flow through a packed column can be used as a basis to investigate the effects of selected important parameters on the pressure drop of a packed bed. The reference process operating conditions were selected and only one parameter was changed at a time. In general, the pressure profiles as shown in Figs. 6 to 8 were observed to be maximum at the initial stage and remained constant as the fluid flow through the packed bed. However, a gradual decrease in pressure occurred as the fluid flow reaches and passing through the adsorbent until it reaches zero and remained at zero as the fluid flow away from the adsorbent.

Effect of Particle Size on Pressure Drop

Figure 6 indicates that when particle size increases, there is a decrease in the pressure drop of the fluid flowing through the packed bed. This is due to the fact that, when the porous particle size increases, the remaining surface area of the bed decreases. In the same way, the decrease in surface area leads to reduction in the resistance of fluid flow and thereby resulted in a decrease in pressure drop of fluid flowing through the packed bed. This variation was also observed by Mayerhofer *et al.* (2011) and Abbas (2009).

Effect of Porosity on Pressure Drop

Fig. 7 shows that an increase in porosity leads to a decrease in the pressure of hydrogen flow through the packed bed. For example, at porosity of 0.35 the pressure drop is 4169260 Pa/m. However, when the porosity increased to 0.7, the pressure drop is 300036 Pa/m. The increase in porosity implies that the void fraction between particles becomes larger and this leads to less resistance to fluid flow through the bed. This result is in agreement with previous work done by Abbas (2009) and Koushik *et al.* (2015).

Effect of Velocity on Pressure Drop

Fig. 8 shows that an increase in velocity result to increase in pressure drop while a decrease in velocity leads to decrease in pressure drop. At a fluid velocity of 0.5 m the pressure drop per unit length was 39849.6 Pa/m. But, at a velocity of 5 m/s, the pressure drop per unit length increased to 636378 Pa/m. This trend was observed when considering the pressure drop of different velocities of 1, 2 3 and 4 m/s as shown in Fig. 8. This observation is in agreement with the works of Mohammadikah *et al.* (2014), Mayerhofer *et al.* (2011) and Abbas (2009).

Conclusion

CFD simulation of hydrogen gas flow in a packed bed was successfully carried out using ANSYS Fluent package and effect of particle size, porosity and fluid velocity parameters on the pressure drop profile investigated. The simulation results compared favourably with the theoretical data obtained using Ergun's equation. CFD results revealed that particle size and porosity were observed to be inversely proportion to the pressure drop of hydrogen gas flow in a packed bed. However, the fluid velocity has a direct effect on pressure drop of fluid flowing through a packed bed system. This study demonstrates that CFD can be effectively used to predict the pressure drop of a fluid in a packed bed.

References

Abbass, M. N. (2009). Estimated equations for water flow through packed of multi-size Particles, *Al-Qadisiya Journal for Engineering Sciences*, Vol. 2, No. 4, 1-22

ANSYS Fluent (2011). ANSYS Fluent 14.0 Users/Tutorial Guide, Modelling flow through porous media, Southpointe, Canonsburg, USA. 1-25

Baker, M. J. (2011). CFD simulation of flow through packed beds using the finite volume technique, unpublished PhD thesis, School of Engineering. University of Exeter, United Kingdom.

Geankoplis, C. J. (2003) *Transport Process and Unit Operations.* 4th ed chapter 3 Prentice Hall: New Jersey.

Koushik, G.S and Panneer, R. (2015), Design and simulation of a hollow cylindrical ceramic air filter using finite volume technique, *Indian journal of science and technology*, Vol. 8, No. 23, 1-8.

Kruger, J. H., Toit, C. G. D and Vandermerwe, W. J. S. (2015). Numerical validation packed beds. *Eleventh international Conference on CFD in the mineral and process industries,* South Whalf, Melbourne, Astralia. 1-7.

Mayerhofer, M.; Parmentier, N.; Jeanmart, H and Helsen, L. (2011). Experimental investigation of pressure drop in packed beds of irregular shaped wood particles. Powder Technology, Vol. 205, No. 1, 30-35, doi:10.1016.powtec.2010.08.006.

Mohammadikah, R.; Abghari, Z.; Sorrod, G., and Ahmadi., M. M. (2014). Improvement of Hydrodynamics performance of Naphta Catalytic Reforming Reactors using CFD. *Journal of Research Institute of Petroleum Industry (RIPI), Vol.* 33, No. 3, 63-76.

Mousazadeh, F (2013). Hot spot formation in trickle bed reactors, unpublished master's thesis, Department of Chemical Engineering. Amirkabir University of Technology, Tehran.

Niaei, A.; Salari, D and Hosseini, S.A., (2009). CFD Simulation of Catalytic Combustion of Benzene, *Iranian Journal of Chemical Engineering,* Vol. 6, No. 4, 34-43.

Pandey, A. K., (2011). A Computational Fluid Dynamics Study of Fluid Flow and Heat Transfer in a Micro channel, unpublished master's thesis, Department of Chemical Engineering, National Institute of Technology, Rourkela, India

Qasim, A.; Adullah, M. Z.; Keong, L. K. and Yusup, S. (2014). Computational Fluid Dynamics Simulation of CO_2 Adsorption on Nanoporous Activated Carbon: Effect of Feed Velocity. *Journal of Applied Science and Agriculture*, Vol. 9, No. 18, 163-169.

Ramchandra, P.G. (2005). Flow modelling and mixing in packed bed reactor, unpublished Doctorate thesis, Department of Chemical Engineering. Indian Institute of Technology Bombay.

Theron, W.G .J. (2011). Numerical analysis of the flow distribution within packed columns, unpublished master's thesis, Department of Mechanical and Nuclear Engineering North-West University, Potchefstroom, South Africa.

Versteeg, H. K. and Malalalsekera, W (2007), An introduction to computational fluid dynamics: the finite volume method, Harlow Prentice Hall, Essex, England.

White, J. (2016). CFD Simulation and Microscopic study of a Solitary Spherical Porous Adsorbent. *School of Engineering Journal*, Birmingham City University, Birmingham.2-15, doi:10.20944/preprints201608.0023.v1.

Zabaleta, A.G. (2007). Computational fluid dynamics Studies in heat and mass transfer studies phenomena in packed bed extraction and reaction equipment, unpublished Phd thesis, Department of Chemical Process Engineering, Universitat Polytechnica de Catalunya.http://hdl.handle.net/2117/93766