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CFD SIMULATION OF BENZENE ADSORPTION ON PISTACHIO ACTIVATED CARBON POROUS MEDIA

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ABSTRACT

In this work, a combination of computational fluid dynamics (CFD) and porous media model was applied to simulate the benzene adsorption on activated carbon and the flow fields in a porous media. The three dimensional unsteady state the gas flow was modeled by using the laminar one phase flow equations in conjunction with the mass transfer equation. The adsorption rate on solid phase was implemented to the model by a user defined source. The model was validated by comparing the simulated breakthrough curves by experimental data. After the validation of the model, the effects of the operating conditions such as benzene concentration, gas flow rate and other parameters on the breakthrough curve and adsorption capacity were studied. The results of CFD model and experiments revealed that the total adsorption time was increased when the gas flow rate and inlet benzene concentration decreased. The results of flow field revealed that increasing the gas flow rate or bed porosity caused the pressure drop decreased.

Keywords: CFD simulation, porous media, benzene adsorption, activated carbon.

1. INTRODUCTION

The common chemical pollutants that must be removed from the air are volatile organic components (VOCs) such as benzene, toluene and xylene. The main VOCs sources are manufacturing industries, petrochemical industries and indoor sources such as solvents used in the production of building materials (paint, carpets, plastic). Most of these components are toxic or have harmful effects on environment. The VOCs are photo-chemically sensitive and in the presence of nitrogen oxides and sunlight form ozone and other toxic products (the main cause of concerns are the ground level of ozone and carcinogenic smog). With respect to these effects worldwide, the current legislation for environmental and human health protection is focused on the VOCs emissions reduction (Faisal et al., 2015; Valenciano et al. 2015; Kristaet al., 2015).

There are several methods for destruction or recovery of VOCs such as condensation, adsorption, catalytic oxidation and thermal oxidation methods. Science the most of VOCs are valuable solvents, then the methods that can recovery these solvents are preferred. Adsorption due to easy and low cost operation, high efficiency and versatility is an interesting physical non destruction method for removal air pollutants. Based on the interaction between adsorbate and adsorbent, the adsorption process is classified into two types, physical and chemical adsorption. In the physical adsorption VOC molecules attached to adsorbent surface by weak Van Der Waals forces and the adsorption heat is low, then the adsorption equilibrium is reversible (Ozturk et al., 2006; Berenjian et al., 2012; Swetha et al., 2016).

Choosing the type of adsorbent is a key parameter in the adsorption process. The adsorbent must be a solid porous material with high surface area and a relatively larger pore network for molecules transport. Activated carbon duo to vast infrastructure of pores and micro pores has large specific surface area.

At industrial applications such as solvent recovery plant, solvent laden air passes through an activated bed and solvent adsorbed on the carbon surface. Initially, the VOC is completely adsorbed and thus concentration the VOC in out flow is zero. But at later times that the total treated gas volume increases, part of carbon bed gets saturated and not adsorbs more VOC. At this time, the concentration of VOC in out flow increases. Finally, when the total available pores surfaces are occupied by VOC, the outlet concentration is equal to inlet concentration and total carbon bed is saturated. For recovery the carbon for reuse, the adsorbed solvent molecules must be realized from carbon surface (Sona et al., 2016; Mirzaei et al., 2016; Wetha et al., 2016).

The laboratory adsorption experiments must be done to determine the adsorption equilibrium and adsorption kinetics. The adsorption equilibrium is obtained isothermally at bath conditions and from the results of this, a suitable adsorbent is selected and then breakthrough times are obtained from kinetic experiments (Debasish et al., 2006; Gil et al., 2014; Kim et al., 2006). Breakthrough curve (outlet concentration/inlet concentration ratio versus time) and adsorption isotherm are used to scale up the adsorption column (Lin et al.2011).

Design an industrial column adsorption depends on many factors as gas flow rate, temperature, concentration and others parameter, so do tests that determine the effects of all of these parameters are costly and time consuming. In the last two decades, numerical modeling and computational fluid dynamics (CFD) have shown great potential as powerful and cost-efficient tools for scale up and optimization of the adsorption column and improve future designs for the adsorption process. These tools enable to prediction of future events and can reveal which factors in a real system are most important from a sensitivity point of view.

All adsorphon models that predict the breakthrough curves are based on adsorbate mass balance. The mass balance is a function of system fluid dynamics, the mechanism of adsorbate mass transfer, the adsorption energy, the adsorption equilibrium and boundary and initial conditions (Li et al. 2010).

The mathematical modeling or a CFD simulation can be developed to predict the flow field and species transport in a porous media. Many

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researchers presented numerical models or CFD simulations for porous materials (Bhatti et al., 2019 and Bhatti et al., 2020).

In principle, adsorption on activated carbon can be implemented as source term into governing flow equation. In the last years, CFD has been used more and more to calculate flow characteristics in packed beds (Jafari et al., 2011; Wei et al., 2011; 1., Asendrych et al., 2003). In the simulation of the adsorption beds, the rate of adsorption/desorption must be added to CFD code. Several models exit for adsorption/desorption in packed bed, such as pore diffusion model, linear driving force model (LDF) and etc. several researchers showed that LDF model is suitable for prediction of gas adsorption in a fixed bed column (Das et al., 2014, Nouh et al., 2010).In present study, the mass transfer between two phases was simulated using LDF.

Only limited studies on the CFD simulation of gas adsorption in the packed bed have been carried out and so far there is no published study on the adsorption of VOC by pistachio shell based activated carbon under dynamic conditions.

Science VOC removal is very important for human health care or recovery of valuable solvents and with the roll of CFD simulation in process optimization, in this study the adsorption of benzene on activated carbon was simulated. The main objectives of this study are as follow:

- Experimental study of benzene removal by pistachio shell based activated carbon at dynamic condition.
- CFD modeling of the hydrodynamic and adsorption phenomena for benzene in the adsorption column filled with pistachio shell based activated carbon.
- In order to determine the operating condition effects on benzene adsorption, the simulations run and experimental tests were done at several operating conditions.

The results of this research can be used for scale up and optimization of VOCs removal process by activated carbon by using CFD tool.

2. MATERIAL AND METHODS

2.1. Adsorbent

In this research, activated carbon obtained from pistachio shell was used as an adsorbent. Activated carbon (AC) is boiled in distilled water for 1 hour before use then washed with deionized water and finally dried in oven at 120 ℃ for 4 hours. Then, to determine the surface area, The BET analyze was done and surface area of AC was 850 m^2/gr with micro and nano pores. The surface structure of the AC was determined by scanning electron microscope (SEM). In figure 1 SEM image of activated carbon was shown.
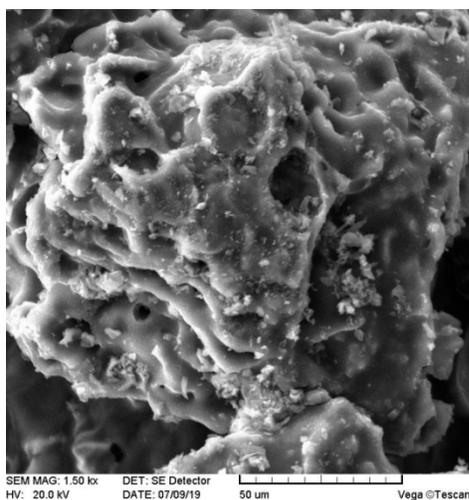
Fig. 1 The SEM image of activated carbon

2.2. Adsorbate

The adsorption on activated carbon is appropriate for recovery of VOC with low molecular weight, 43-150. The smaller compounds on the carbon surface are not well absorbed and heavier compounds during recovery cannot be removed from the surface. One of these VOC components is benzene. Some industries use benzene to make other chemical materials including plastics, resins, nylon and synthetic fibers. A major source of benzene exposure is tobacco smoke and human exposure to benzene has been associated with a range of acute and long-term adverse health effects and diseases, including cancer and anaemia.

2.3. Adsorption tests

Figure 2 shows the experimental setup that used in this research. The dry N2 were bubbled through a gas washing bottle containing pure benzene and collected in a cylinder. In order to obtain desired benzene concentration in gas flow, the gas washing was filled by a specified amount of liquid benzene (calculated based on the volume and pressure of cylinder) and the N2 passed through the benzene until the total benzene evaporated into N2 gas and the pressure of gas in the collecting cylinder reached to desired value. All the gas flow rates were controlled with mass flow controller (MFC).

The adsorption tests were done at isothermal condition in a Pyrex double tube fixed bed reactor, 0.7 cm inner diameter. In each test the activated carbon (1 gr) was placed inside the inner tube and in order to keep the temperature constant, outer tube was connected to a refrigerator unit and water with desired temperature was recycled in it. The several operating conditions under which adsorption tests were carried out were concentration of benzene (1000, 700 ppm) and gas flow rate (100 and 200 ml/min). The adsorption tests were done continuously until the outlet concentration was equal to the inlet concentration.

The concentration of benzene in the inlet and outlet flow were determined by gas chromatograph (GC, Agilent USA) equipped with a flame ionized detector, FID. Before the experiments, the GC was calibrated by using three points calibration for benzene vapor concentration. The calibration points were 1000, 700 and 300 ppm and related to the peak area output of the GC. Linear regression was used to relate GC peak area output to benzene concentration.
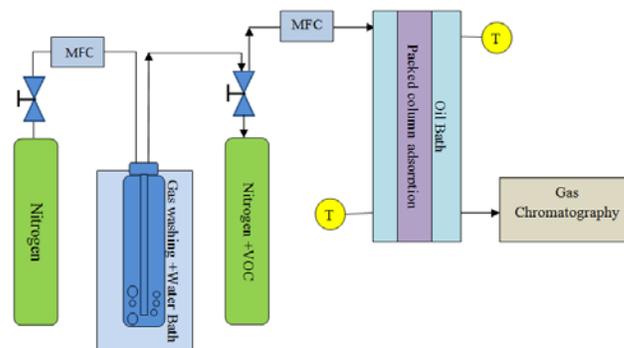
Fig. 2 Experimental set up for adsorption tests

3. CFD SIMULATION

3.1. Governing equations:

The porous media model is applicable for vast range of one and multi phase flows such as flow in the packed beds, filter papers and perforated plates. When using this model, a domain defined that the porous model used in it and flow pressure drop calculated in this regime. Heat transfer in the porous domain calculated by local equilibrium assumption between porous media and fluid flow. The following assumptions were considered in the presented study:

- – The linear driving force model was selected for mass transfer from gas to carbon.
- – The concentrations of gas bulk and pellet surface are at equilibrium instantaneously
- – The bed porosity was uniform
- – The temperature was constant (according to literatures, the adsorption heat of benzene on activated carbon is low)

3.1.1. Continuity equation

The mass conservation equation can write as (Nouh et al., 2010):

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

Where

$$S_m = \frac{1-\varepsilon}{\varepsilon} \rho_p \frac{\partial q_i}{\partial t} \tag{2}$$

where $\partial q_i / \partial t$ is the adsorption/desorption rate of ith species.

3.1.2. Momentum equation

The conservation momentum equation for one phase flow is (Nouh et al., 2010):

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla.(\rho \vec{v}\vec{v}) = -\nabla p + \nabla.(\bar{\bar{\tau}}) + \rho \vec{g} + \vec{F} \tag{3}$$

where $p, \bar{\bar{\tau}}, \rho\vec{g}, \vec{F}$ denoted static pressure, stress tensor, body gravity force and external forces, respectively. Also $\vec{F}$ contains other source terms such as porous media sources and sources that defined by users. Stress tensor defined as:

$$\bar{\bar{\tau}} = \mu\left[(\nabla\vec{v} + \nabla\vec{v}^T) - \frac{2}{3}\nabla.\vec{v}I\right] \tag{4}$$

where μ is molecular viscosity. The porous media modeled by adding a momentum source term S_i to the standard fluid flow equations. This source term consists of two parts, viscose loss term and inertial loss term.

$$S_{i,prous\ media} = -\left(\sum_{j=1}^{3} D_{ij}\mu v_j + \sum_{j=1}^{3} C_{ij}\frac{1}{2}\rho|v|v_j\right) \tag{5}$$

where S_i is the source term for i^{th} momentum equation. This sink of momentum Contributes to the porous cell pressure gradient. This produces a pressure drop that proportional to fluid velocity in the cell. In the case of homogeneous porous media S_i can be written as:

$$S_{i,prous\ media} = -\left(\frac{\mu}{\alpha}v_i + C_2\frac{1}{2}\rho|v|v_i\right) \tag{6}$$

where

$$C_2 = \frac{1.75}{D_p}\frac{(1-\varepsilon)}{\varepsilon} \quad and \quad \alpha = \frac{D_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2} \tag{7}$$

where α and C_2 are the permeability and the inertial resistance factor. In the laminar flow in porous media, the pressure drop is proportional to the velocity and C_2 considered zero. With neglecting from convective acceleration and diffusion, the porous media model reduced to Darcy low:

$$\nabla p = -\left(\frac{\mu}{\alpha}\vec{v}\right) \tag{8}$$

When there is species transfer in the system, the extra momentum source term appears in the momentum equations:

$$S_{i,species\ transfer} = -\frac{1-\varepsilon}{\varepsilon}\rho_p v_i \frac{\partial q_i}{\partial t} \tag{9}$$

3.1.3. The species transport equation

When the mass transfer or chemical reaction exist in the system, the conservation equations for chemical species must be considered with mass and momentum conservation equations. This equation, that predicts the local concentration of any species C_i during the solution, is a convective-diffusion equation for component ith and expressed as (Nouh et al., 2010):

$$\frac{\partial}{\partial t}(C_i) + \nabla.(C_i\vec{v}) = -\nabla\vec{J}_i + R_i + S_i + R \tag{10}$$

where C_i is local concentration, R_i is net homogeneous production rate by chemical reaction, S_i rate of addition mass by dispersed phase and any other sources, $\vec{J}_i$ is diffusion flux duo to concentration gradient and R is heterogeneous reaction rate. In this study, R_i and R were considered zero and S_i was considered as a sink term (adsorption/ desorption isotherm) that implemented to soft ware as a user defined source (Dung et al., 2015).

$$S_i = \left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{\partial q_i}{\partial t} \tag{11}$$

The adsorption rate $\partial q_i / \partial t$ was obtained based on the linear driving force model (LDF) as shown:

$$\frac{\partial q_i}{\partial t} = \left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{k_i a}{\rho_s}\left(C_i - C_i^p\right) \tag{12}$$

where C_i and C_i^p are benzene concentration in the gas bulk and pellet concentration respectively.
The pellet concentration C_i^p is described by Langmuir model.

$$q_i = \frac{q_{max}K_A C_A}{1+K_A C_A} \tag{13}$$

where q_{max} is the adsorbent maximum capacity concentration and K_A is adsorption equilibrium constant. In this research q_{max} and K_A are considered as fitting parameters.

In all types of CFD modeling there are some factors that determine the difficulty of modeling. In an adsorption packed bed the amount of packing and the narrow region between them makes its modeling more complicated. One way of solving this prob-lem is to model a single granule of silica gel in CAD software

In this paper The adsorption rate $\partial q_i / \partial t$ was (the equations 12) was implemented to CFD code by user defined source and q_{max} and K_A selected as fitting parameters.

3.2. Geometry and boundary conditions

The geometry of the adsorption bed was a tubular bed with 0.7 cm inner diameter and 5 cm high. The mixture of gas, nitrogen and benzene vapor, inter from top of the bed and out from down of bed. The active section of bed that filled with adsorbent was defined as porous domain. The geometry was built by using Ansys design modeler and was meshed. The velocity inlet and outlet pressure boundary conditions were chosen at inlet and out let, respectively. At wall of the bed, constant temperature thermal boundary condition was used. The geometry and boundary conditions that were used in the CFD model was shown in Fig. 3.
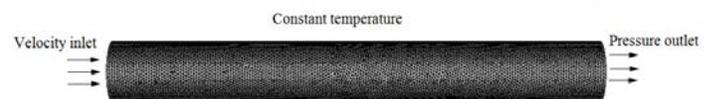
Fig. 3 The geometry and boundary conditions

3.3. Calculation Procedure

The governing equations were solved by using commercial Ansys Fluent software 18. Second order upwind discretization scheme was used for the momentum, species and energy. The grid independency test was carried out with three different three-dimensional meshes, which contained 800,000, 1,200,000 and 2,300,000 cells respectively. Table 2 shows a comparison of the total adsorption time with different cells. As one can see in this figure, increasing the number of cells from 1,200,000 to 2,300,000 did not show important changes in the results. Therefore, the 1,200,000 cells were used as a grid-independent case for the computations.

Table 1. % errors between simulation results of total time adsorption with different cells and experimental data

Number cells	$\dfrac{time_{sim} - time_{exp}}{time_{exp}} \times 100$
800,000	14
1,200,000	9
2,300,000	8.5

4. RESULTS AND DISCUSSION

4.1. Validation of the model

At first, in order to validate CFD model, the simulation results were compared with experimental data and the results were presented in figure 4. In this figure the adsorption capacities (mg adsorbed benzene/gr carbon) of activated carbon obtained by CFD model together with the corresponding experimental data as function of gas flow rate were presented. As can see, the model predicts a few higher adsorption capacities. At isothermal condition, the benzene adsorption controlled by the three mechanisms: the film mass transfer of benzene from the gas bulk to carbon surface, the benzene diffusion in carbon pores and the adsorption/ desorption inside the pores. In the proposed model the first and third mechanism were considered and diffusion pore resistance was neglected (semi homogenous model), then the adsorption resistance was decreased and more amount of benzene adsorbs on carbon surface. The mean difference between CFD model results and experimental data were less than 7% and therefore proposed model is able to predict the adsorption behavior reasonably. Based on this good agreement, this CFD model can be used to determine the effects of operating condition on benzene adsorption performance
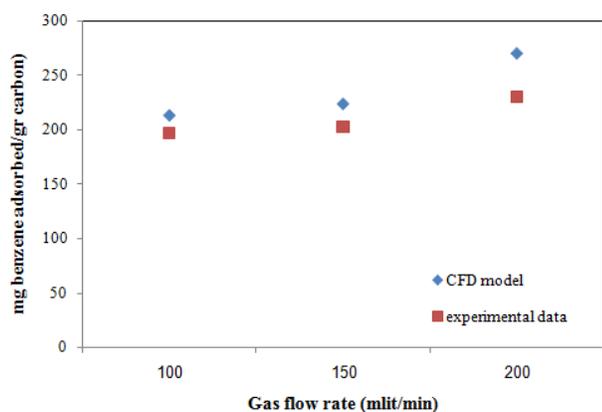
Fig. 4 Adsorption capacity versus gas flow rate (C=1000 ppm, T=25)

4.2. Flow hydrodynamic

The hydrodynamics effect on mass transfer and then adsorption capacity of benzene. Figures 5 and 6 showed the axial distributions of static pressure and gas velocity along the adsorption bed respectively at two bed porosity. As can see from this figure, the pressure significantly drops in the porous zone duo to high resistance of the flow in this media. The velocity of gas keeps constant in the porous media and the gas is uniformly distributed across all cross section. Figure 6 shows that with increase the bed void fraction the available area for gas flow increases and then the gas velocity decreases. Additional, the flow resistance decreases and therefore the pressure drop decreases also.

In order to determine the effect of gas velocity on adsorption performance, the adsorption capacity at two states (two porosity) was determined (Q=200 L/min, C=1000ppm). The CFD results showed that by increment the bed porosity from 0.45 to 0.5, duo to decrease the total gas residence time in the bed, the benzene adsorption capacity decreased from 439 to 398.2 (mg benzene/g carbon).
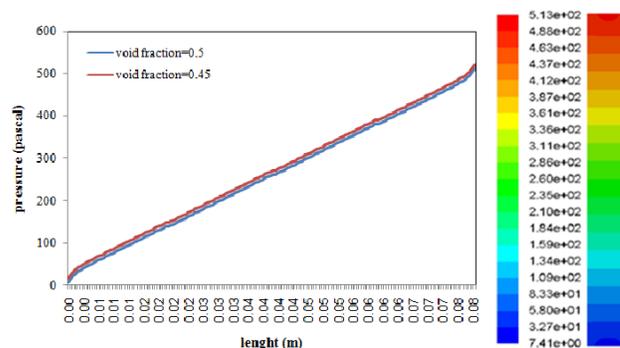
Fig. 5 The axial static pressure distribution along the adsorption bed (C=1000 ppm, T=25 ℃ and Q=200 ml/min)
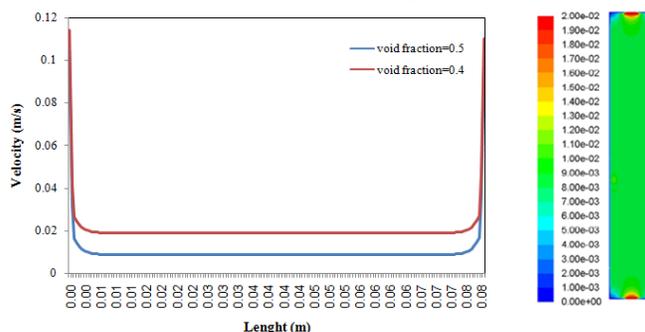
Fig. 6 The axial velocity distribution along the adsorption bed (C=1000 ppm, T=25 ℃ and Q=200 ml/min)

4.3. Benzene adsorption

4.3.1. The effect of gas velocity

In order to determine the effect of gas flow rate on breakthrough curve and adsorption capacity, the experiments and simulation runs were done at two gas flow rates (constant temperature 25 ℃ and constant inlet benzene concentration 1000 ppm). Figure 7 shows the adsorption breakthrough curves of benzene through the packed bed column that contained 1 gram of activated carbon. It is clear that reduction of the gas velocity caused that the breakpoint appears later and adsorption capacity slightly reduced. As mentioned above, benzene most transfer from the gas bulk to carbon surface by film mass transfer and k_m (film mass transfer coefficient) is a function of Reynolds number. With increase the gas flow rate from 150 to 200 the Reynolds number increases from 0.2×10^{-6} to 0.25×10^{-6} and therefore k_m increased little and then adsorption capacity increased. In other hand, by increment the inlet gas velocity, the gas residence time in the adsorption bed decreased. Then by respect to the presented results in figure 7, the effect of mass transfer coefficient dominated to the residence time and at higher inlet gas

velocity (from 150 to 200 L/min), the adsorption capacity increased little from 425.2 to 439.

Additionally, in figure 7 the experimental data and CFD results were compared and good agreement existed between them. The mean error of results was about % 9.5, then the proposed model is able to predict the adsorption behavior reasonably.
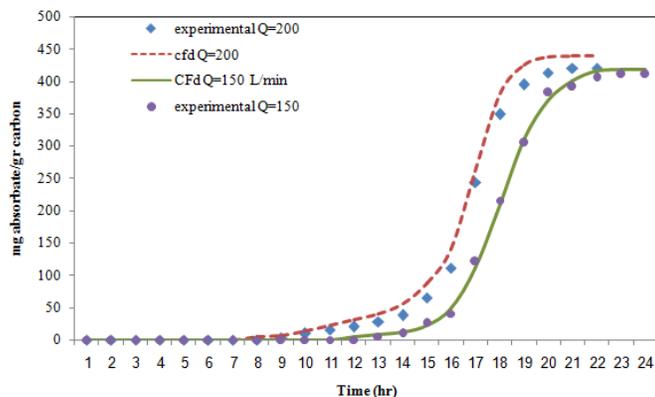
Fig. 7 The breakthrough curve at different gas flow rate (C=1000 ppm, T=25 ℃, 1 gr of activated carbon)

The counters of mass fraction of benzene along the adsorption bed were shown in figure 8 at different times. As can see from this figure, at initial times the concentration of benzene at bed outlet is zero and this means that total benzene was adsorbed on carbon surface and with over time the bed is saturated and concentration of benzene was increased at outlet. In this proposed CFD model K_A (adsorption /desorption rate constant) and q_{max} (the maximum capacity) were considered as adjustable parameters and were calculated in our previous work. These counters proved that the radial velocity and radial concentration distributions not exist.
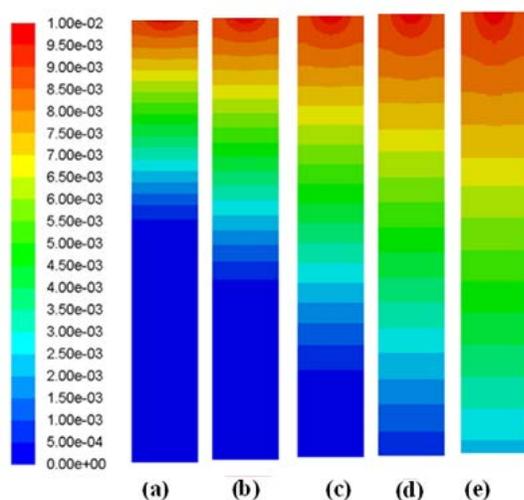
Fig. 8 The counters of benzene mass fraction at different time a) 7 hr, b) 13 hr c) 19 hr d)23 hr (C=1000 ppm, T=25 ℃ and Q=200 ml/min)

4.3.2. The effect of inlet benzene concentration

The effect of benzene concentration on breakthrough curve was studied by change the gas inlet concentration. The adsorption experiments and run simulations were performed at two benzene concentration 100 and 700 ppm (the temperature and gas flow rate were kept constant at 25 ℃ and 200 ml/min respectively). In figure 9 the breakthrough curves of adsorption benzene at two different concentrations were compared with

corresponding CFD breakthrough curve. As this figure shows, the breakpoint increases at lower inlet concentration (from 7 to 13 hours with decrease the inlet concentration from 1000 to 700 ppm) then at low concentration, the present adsorbent can be used for long time with high separation efficiency. At higher benzene concentration, the carbon bed saturated sooner and equilibrium was achieved at shorter time.
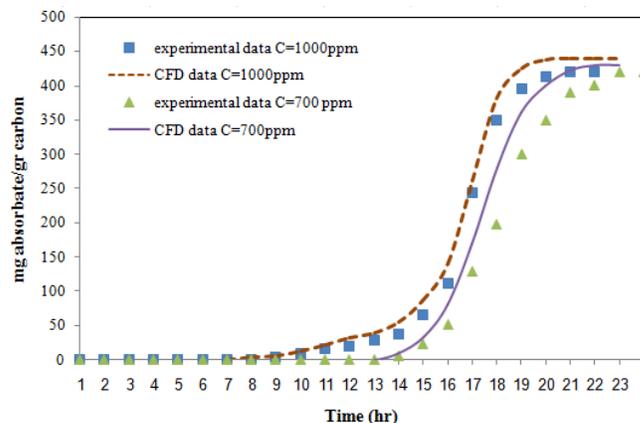
Fig. 9 The breakthrough curve at different benzene concentration (C=1000 ppm, T=25 ℃, 1 gr of activated carbon)

4.3.3. The effect of BET area

The above results show that the proposed CFD model is able to predict the adsorption behavior reasonably. Then this model is used to study the effect of adsorbent BET area on adsorption capacity. For this purpose the simulation runs were performed at three different BET area (850, 950 and 1100 (m^2/m^3), C=1000 ppm, Q=200 ml/min) and the obtained results were shown in figure 10. As evident from this figure, when BET area increases from 850 to 950 (m^2/m^3), the adsorption capacity increases from 439 to 510. This is duo to that more surface area is available to benzene adsorption.
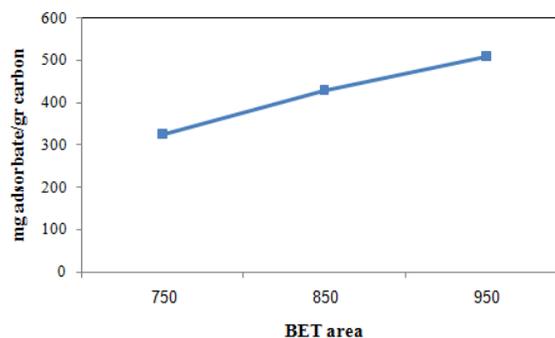
Fig. 10 The adsorption capacity versus BET area (C=1000 ppm, T=25 ℃ and Q=200 ml/min)

5. CONCLUSION

Science the CFD is a powerful tool for design and optimization of process equipments and the CFD studies related to adsorption of VOC in a fixed bed column have been found to be limited, in this study a CFD model was presented for the adsorption of benzene vapor in a fixed bed reactor by activated carbon. The proposed model was an unsteady state three-dimensional model that the porous media model was used in it for study the flow behavior in adsorbent bed.

The results of the research are summarized as follows:

- The results of experimental tests showed that Pistachio shell based activated carbon is a potential adsorbent for benzene removal.
- The predicted breakthrough curves obtained by CFD model were found to be in good agreement with the experimental data.
- By increment the inlet gas velocity from 150 to 200 (L/min), the adsorption capacity increased (from 419 to 439 mg benzene/g carbon).
- Among all the operational parameters, the BET area had higher impact on adsorption capacity and with increase the BET area from from 850 to 950 (m2/m3), the adsorption capacity increases from 439 to 510.

The results of this study implied that CFD tool can be used to predict the behavior of industrial fixed bed adsorption process at various operating conditions reasonably and then optimize the process and equipment. As respects to that the proposed CFD model in this study is a semi-homogeneous model (the mass transfer and distribution benzene concentration in the solid phase no considered), developing a heterogeneous model can be very beneficial to know more aspects of adsorbent behavior.

NOMENCLATURE

a External surface area per unit volume (m^2/m^3)
C   Concentration (mole/m^3)
D   Diffusivity coefficient (m^2/s)
D_p Particle diameter (m)
g   Gravity acceleration (m^2/s)
K Adsorption equilibrium constant
L   Volumetric gas flow rate (L/min)
P   Particle
p   Pressure (N/m^2)
R   Chemical reaction rate
t   Time (s)
T   Temperature (K)
v   Velocity (m/s)

Greek letters:
ρ   Density (kg/m^3)
ε   Porosity of bed
τ   Stress tensor
μ   Viscosity (Pas)

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