Proceedings of Iran International Aluminum Conference (IIAC2014)
May 25-26, 2014, Tehran, I.R. Iran

Study of separation CO with H_2 on carbon nanotube by monte carlo simulation in aluminum smelter

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Abstract: Co is very toxic gas so separation of this gas is very important .In this study separation of co and h2 Has been studied. Prevent the emission of carbon monoxide in the environment is very important..in this study Lennaed-Jones potential was used for gas-gas and gas-carbon nanotube interactions and the potential parameters for the carbon-gas and carbon-carbon interactions were obtained from the Lorenz-Berthelot combining rules. The study has been done by using the equation state of Virial and finding the second coefficient in Virial equation. Final steps were the inside density, outside density and total density of nanotubes .My calculation.result show that this sepration is possible.

Keywords: “Carbon nanotube, adsorption gas ,monte carlo simulation;”

Introduction

Adsorptive separation of particular gaseous mixtures is a viable industrial process, where one component must be selectively adsorbed on a suitable adsorbent relative to the other. However, the properties of gas mixtures adsorbed in small spaces are quite different from those in bulk phases. Since microporous membranes and adsorbents are routinely used in industrial separation processes, understanding these effects is vital for developing new separation technologies and optimizing currently used techniques. Selectivity in micro porous adsorbents is controlled by a number of factors: the adsorb ate–adsorb ate interactions for like and unlike molecules including the strength of adsorb ate–adsorbent interactions, as well as geometric considerations such as microspore width and the size and shape of the adsorptive species. Most of the studies on adsorptive separation are based on carbon sorbents. Several research groups have carried out experimental studies in this area. Park et al. [1] introduced a new kind of sorbent structure, which arranges activated carbon and zeolite in layers alternatively. Using different selectivity’s of the two sorbents toward gas mixture, hydrogen gas with relatively high purity can be obtained. Raged al. [2] combine 13X-zeolite, _-AL2O3, natural-zeolite, K+-zeolite and Ca2+-zeolite together to maker-purification of nitrogen and oxygen in air. Clarkson [3] studied the effects of different moisture content on the selectivity of carbon sorbents. As discovered by Iijima [4] in 1991, carbon nanotubes can be obtained by rolling up a single layer or multiple layers of graphite basal planes with a definite diameter[5,6]. Carbon nanotubes are now considered as one of the most promising gas separation system. However, to study the adsorption behavior via experiments is difficult because the microscopic properties of porous solids are often hard to determine. The techniques of molecular simulation are ideally

Suited to this study since model microspores and adsorbents can be defined in an unambiguous fashion

on the computer. Gelb et al. [7In this work, grand canonical Monte Carlo (GCMC) method is used to study the adsorptive separation ofthe hydrogen and carbon monoxide in aluminum smelter. Single-walled carbon nanotubes are selected to be the adsorbent. We made a thorough and elaborate study on the effects of the packing geometry of carbon nanotubes on gas separation. To make a more comprehensive work, the influence of temperature as well as pressure on the separation is also studied. The simulation results in this work canbe used to optimize the pore geometry for gas separation at a given pressure and temperature.

Simulation Method

The Monte carlo statistical mechanical simulation were carried out in standard manner using the Metropolis sampling technique in canonical (T,V,N) ensamble.In this work, all of the particles include hydrogen sulfide molecules, and carbon atoms are treated as structureless spheres. Particle-Particle interactions between them are modeled with Lennard-Jones potential located at the mass-center of the particles.In this work, as in the works of many researchers, the cut and shifted Lennard-Jone(LJ) potential was used to represent the interaction between hydrogen sulfide molecules

$$\phi_{ff}(r)=\begin{bmatrix}\phi_{ij}(r)-\phi_{ij}(r_c) & r<r_c\\ 0 & r\geq r_c\end{bmatrix}$$

Where r is the interparticle distance, r_c is the cut off radius, $r_c=5\sigma_{ff}$. ϕ_{ij} is the full LJ potential,

$$\phi_{ij}=4\varepsilon_{ff}\left[\left(\sigma_{ff}/r\right)^{12}-\left(\sigma_{ff}/r\right)^{6}\right]$$

where ε_{ff} and δ_{ff} are the energy and size parameters of the fluid.They are 301.1 and 3.62nm for hydrogen sulfide here,respectively.The interaction between the wall and a hydrogen sulfide molecule is calculated by the site-to-site method[6-16].

$$U_{fw}=4\,\varepsilon_{fw}\sum_{i=1}^{N_f}\sum_{j=1}^{Nsabon}\left[\left(\frac{\sigma_{fw}}{r_{ij}}\right)^{12}-\left(\frac{\sigma_{fw}}{r_{ij}}\right)^{6}\right]$$

Where N_f is the number of hydrogen sulfide gas molecules, N_{carbon} is the number of carbon atoms of the wall of SWNT. ε_{fw} and δ_{fw} are the cross-energy and size parameters, which are obtained from the Lorentz-Berthelot (LB) combining rules.Energy and size parameters of carbon atoms are 28.0 and 0.34nm, respectively[20]. r_{ij} is the distance between a gas hydrogen sulfide molecule and an atom of the wall of SWNT.

Lorentz-Berthelot rules are used to calculate the parameters of interaction between different kinds of particles.In this calculation, all of the particles are regarded as spheres.Interaction among particles are modeled with Lennard-Jones potential acted on the mass center.The initial configuration was generated randomly (Figure1). For a fixed cell, three types of moves were used to generate a markov chain, including moving, creating, and deleting a molecule and make new configurations[]. The three types of moves have the same probability and each has different receiving opportunities.Configurations are accepted when they obey Metropolis's Sampling scheme in proportion to $\exp\left(\frac{-\Delta E}{KT}\right)$ where ΔE is the change of total energy in the system.

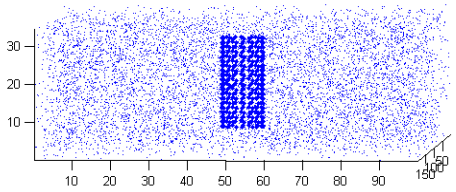

Fig1-

The statistical error have been reported in this work.STDEW is the standard deviation of the calculated average in the simulation of eight number is 0.64% (simulatin error).The dimensions of simulation cell is $(200\times100\times34.5)A^{\circ}$. We considered single-walled armchiar $(8,8)$ nanotubes with open edge(Figure2).The number of carbon atom is 320.The diameters of the nanotubes is $10.854A^{\circ}$, and the averge bond length is $24A^{\circ}$ respectively.The number of molecules gas calculated by virial equation of state and input to the GCMC calculation. The equation of state of real gases is best represented, by the series (equation 3)

$$PV_m=RT\left[1+\frac{B_{(T)}}{V_m}+\frac{C_{(T)}}{V_m^2}+\frac{D_{(T)}}{V_m^3}+\cdots\cdots\cdots\right].$$

Where $B_{(T)}, C_{(T)}$,and $D_{(T)}$ are respectively termed the second, third, and fourth virial coefficients. (P) is the pressure, (V_m) is molar volume, (T) the absolute temperature, and (R) the gas constant[19].

Results and Discussions

Evaluation of separating hydrogen and carbon monoxide

In this study, separation of hydrogen and carbon monoxide, on the nanotube is investigated. Lorentz-Berthelot rules are used to calculate the Potential parameters for the interaction of hydrogen – CO and hydrogen-carbon and CO-carbon Combination of rules Laurent - Berthelot obtained.

H_2		CO		$Carbon\ Nanotube$	
$\sigma_{ii}(nm)$	$\varepsilon_{ii}k_B^{-1}(K)$	$\sigma_{ii}(nm)$	$\varepsilon_{ii}k_B^{-1}(K)$	$\sigma_{ii}(nm)$	$\varepsilon_{ii}k_B^{-1}(K)$
./282	**57/7**	**0/369**	**91/7**	**0/34**	**28/2**

Table 1-potential parameters of the fluid (gas) and nanotube

$$\sigma_{ij} = (\sigma_{ii} + \sigma_{ij})/2$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ij}\varepsilon_{jj}}$$

	$\varepsilon_{iJ} k_B^{-1}(K)$	$\sigma_{ij}(nm)$
$H_2 - Carbon\ Nanotube$	40/88	./311
$H_2 - CO$	73/98	./325
$CO - CarbonNanotube$	50/67	./354

Table 2 - Potential parameters for the interaction of components

-In the first phase of research adsorption of mixture of 33% hydrogen gas and ٪66carbon monoxide

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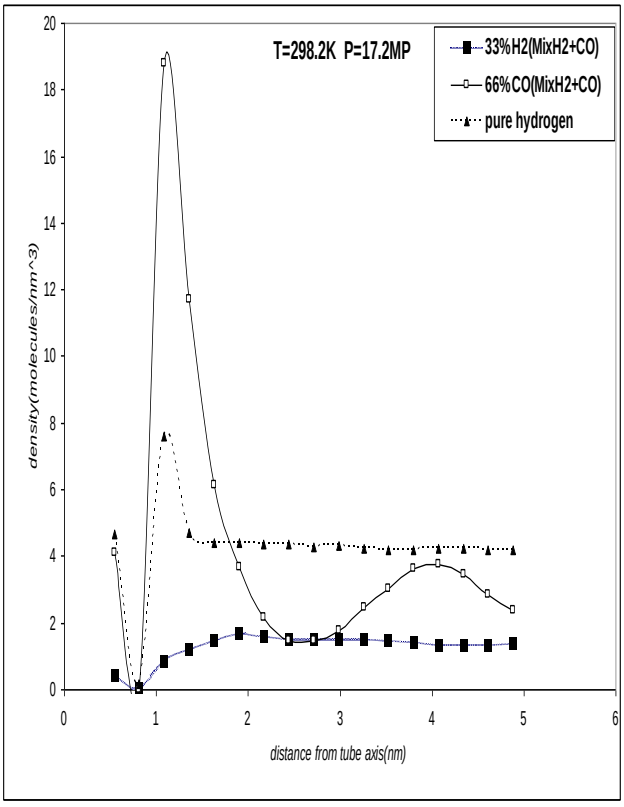

Fig2-Distribution of hydrogen and monoxide carbon gases form the tube axis

According to the figure, we see that the number of moles of hydrogen gas is lower than carbon monoxide.

But the amount of hydrogen gas adsorption more than carbon monoxide adsorbed.This indicates that interactions between the tubes are carbon monoxide is stronger.And as can be seen in Fig. Because of its high interaction between carbon monoxide gas and hydrogen, Hydrogen adsorption is greatly reduced compared to the pure state.Since fixed nanotube diameters considered here probably due to differences in the relative size of two hydrogen molecules and carbon monoxide Separated with high separation factor.The reason is that the interaction of hydrogen with carbon monoxide molecules

More severe than the interaction with hydrogen – hydrogen, Therefore is slow to adsorb hydrogen gas.inside density, outside density and total density of hydrogen and carbon monoxide gases adsorbed on carbon nanotubesAccording to the figure, we see that sincePresent Of carbon monoxide in the composition with hydrogen is twice.But the total amount of adsorbed CO is estimated treble hydrogen.

The second phase of the study

In the second phase of this study, adsorption mixed of 66% hydrogen with 33% hydrogen was studiedAs we see in Figure Here, because of the greater mole percent adsorption of Carbon monoxide in composition, Occurs with greater intensity.in this There is a strong absorption peak ofcarbonmonoxide around the nanotube axis, lack of hydrogen absorption peak in this region, the possibility of separating the gas from the two together allows.

	Total density $molecules/nm^3$	Out side density $molecules/nm^3$	Inside density $molecules/nm^3$
$0.66 mole H_2$	0/45	2/48	2/34
$0.33 mole CO$	./22	6/08	6/07

Table3-inside density, outside density and total density of hydrogen and carbon monoxide gases adsorbed on carbon nanotubes

The review of the previous table, this table comes to the conclusion that each of these molecules in combination with increasing mole percent of the total density of the nanotube axis is greater.

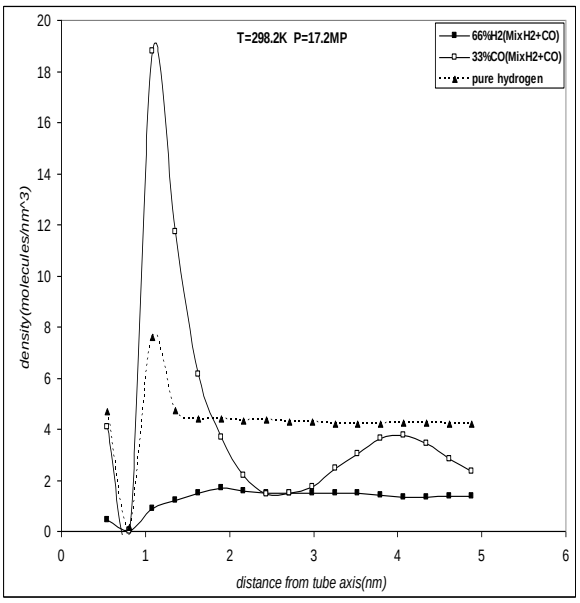

Fig3-Distribution of hydrogen and monoxide carbon gases form the tube axis

Conclusion

. Results show that this separation of carbon monoxide with hydrogen by carbon nanao tube is possible.

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