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Applying Nano Technology To Remove Toxic H2S Gaze Compounds From Exhaust Gases In Primary Aluminium Industry (Monte Carlo Simulation)

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Keywords: Carbon nanotube, adsorption gas ,Monte carlo simulation

Abstract

Dealing with the exhaust gases from aluminium smelters is still an interesting subject for investigation. The amount of H2S in aluminium reduction cells is enough to produce H2S gaze. Immediate removal of the highly toxic H2S gases makes FTP (Fume Treatment Plant) to just deal with fluoric gases such as HF. Due to the capability of nanotubes in adsorbing gases, this study has been conducted to figure out the adsorption of H_2S on (8,8) armchair carbon nanotubes (CNTs). 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 calculation.

Keywords: Carbon nanotube, adsorption gas ,monte carlo simulation

Introduction

In 1991, Iijima announced the discovery of multiwall carbon nanotubes as a byproduct in fullerene production[1-3]. Since then, great efforts were made to improve the yield during the preparation and purification. Single-walled carbon nanotubes (SWNT) are available since 1992 in enough quantities to be studied, and immediately attracted attention because of potential technological applications and also from basic research perspective because it was the first from of carbon that could provide physical realizations of ideal systems.

Single-walled carbon nanotubes could be considered as the result of bisecting a C_{60} molecule at the equator and the two resulting hemispheres are joined with a cylindrical tube one monolayer thick and with the same diameter as C_{60}. If the C_{60} molecule is bisected normal to a 5-fold axis, an armchair tubule is obtained, whereas if the bisection is made normal to a 3-axis, a zigzag type tubule is obtained. Other chiral tables can be formed with a screw axis along the axis of the table. Carbon nanotubes can be specified in terms of the table diameter d_t,and chiral angle θ, that define the chiral vector. $c_h = na_1 + ma_2$ .The tube can then be identified using pair of integers (n,m) that define the chiral vector[4].

Carbon nanotubes have been found to assemble in bundles where the tubes are in a hexagonal array with different lengths. Carbon nanotubes have gathered much attention both from fundamental science and technological interests. Very high chemical stability and mechanical strength made the carbon nanotube a very important material in nanotechnology[].Existing theoretical literature suggests that defect-free, pristine carbon nanotubes (CNTs) interact weakly with many gas molecules like H_2O, CO, NH_3, H_2, and so on[5].

In this work, grand canonical Monte Carlo (GCMC) method is used to study the hydrogen sulfide adsorption gas on carbon nanotube.Single-Walled carbon nanotubes are selected to be the adsorbent.To make a comprehensive work, the influence of temperature as well as pressures on the adsorption is also studied.

The simulation results in this work can be used to optimize the hydrogen sulfide adsorption 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.

$$\phi_{ff}(r) = \begin{bmatrix} \phi_{ij}(r) - \phi_{ij}(r_c) & r < r_c \\ 0 & r \geq r_c \end{bmatrix} \quad (1)$$

Where r is the antiparticle 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].

$$U_{fw} = 4\varepsilon_{fw}\sum_{i=1}^{N_f}\sum_{j=1}^{Ncabon}\left[\left(\frac{\sigma_{fw}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{fw}}{r_{ij}}\right)^{6}\right] \quad (2)$$

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.

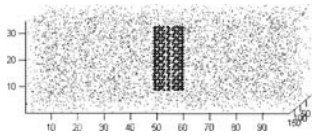

Figure1.initial configuration

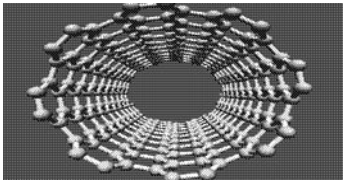

Figure 2.Armchiar (8,8)

To insure good thermodynamical averages, for a single isotherm point typically 5×10^6 moves have been performed to equilibrate the system.for each of five hundred configuration, one configuration is selected, and names snapshot.diagram energy of produced configuration to namber of snapshot show that system reach to the equilibrium.

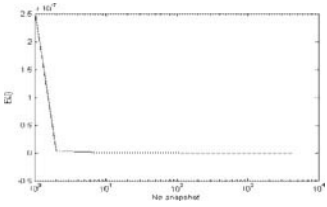

Figure 3.snapshot to percent of abundance

The ensemble average energy of system for second helf of snaphshots is drawen, and initial part is discarded. Because initial part far away to the equilibrium.diagram of energy for second helf, show that,the system reach to equilibrium.

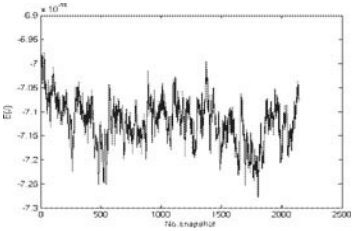

Figure 4.snapshot for second helf to percent of abundance

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 $(200 \times 100 \times 34.5)A^{\circ}$. 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 $10.854\ A^{\circ}$, and the averge bond length is $24\ A^{\circ}$ 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 Discussion

Influence of temperature on hydrogen sulfide adsorption in carbon nanotubes

In this work all simulation has been performed at 310.9, 344, 377, 410K , and 7MP to characterize the adsorption process. For calculation density of hydrogen sulfide adsorption on carbon nanotube, the center of carbon nanotube is selected for zero of Cartesian system.and by make hypothetical cylinder's around of carbon nanotube, inside density of carbon nanotube,out side density of carbon nanotube, total density of carbon nanotube, and amount of difference density to distance from tube axis is calculated.

In Figure 5. show that the total amount of hydrogen sulfide adsorption on single-walled carbon nanotube, increases with low temperature. And amount of density around of tube axis is more then the other space.

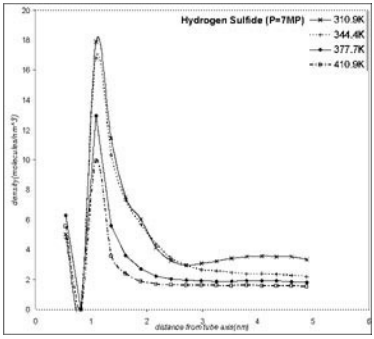

Figure 5.distribution of hydrogen sulfide gas to distance from tube axis

In table1 show that calculated density of inside carbon nanotube,density of out side carbon nanotube, and density of out side carbon nanotube .

$T\ (K)$	310.9	344.4	377.7	410.9
Second virial coefficients $(cm^3/mole)$	-185.5	-145.3	-117.6	-95
Number of gas molecules	1125	1015	926	851
In side density $(molecules/nm^3)$	4.52	6.28	5.73	5.28
Out side density $(molecules/nm^3)$	7.63	4.44	2.92	2.26
Total density $(molecules/nm^3)$	7.44	4.55	3.09	2.45

Table1-density of inside hydrogen sulfide adsorption on carbon nanotube,density of out side hydrogen sulfide on carbon nanotube, and density of total hydrogen sulfide adsorption

It is found that at high temperature, endohedral adsorption has higher hydrogen sulfide uptake against the exohedral, while at low temperature,exohedral adsorption exceeds the endohedral.This indicates that in applications of SWNTs for adsorption hydrogen sulfide gas at low temperature,exohedral adsorption or adsorption on outer surfaces of SWNTs might be significant and comparable with that inside the tubes.This suggestes that introduction of exohedral adsorption would improve adsorption at low tempeature, while introduction of endohedral adsorption would improve adsorption at high temperature.In figure .5, the total amount adsorotion increases with perssure

Figure 5 show that relation between temperature and amount of hydrogen sulfide adsorption on carbon nanotube.

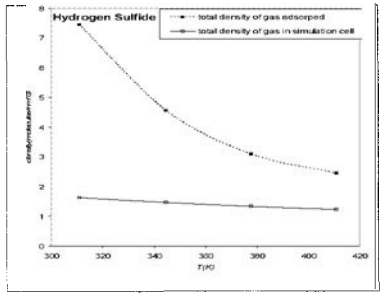

Figure 5. Relation between density of hydrogen sulfide gas and tempreture

Influence of pressure on hydrogen sulfide adsorption in carbon nanotubes

In this work all simulation have been performed at 3, 5, 9,11MP and 277.7K to characterize the adsorption process.
scheme -4 show that the total amount of hydrogen sulfide adsorption on single-walled carbon nanotube, increases with low temperature

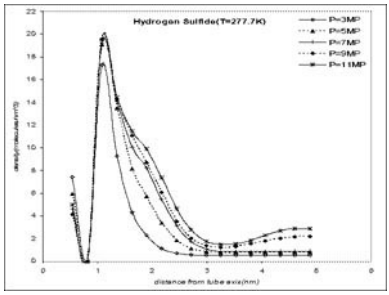

Figure 5.Distribution of hydrogen sulfide gas to distance from tube axis

Table1-density of inside hydrogen sulfide adsorption on carbon nanotube,density of out side hydrogen sulfide on carbon nanotube, and density of total hydrogen sulfide adsorption on carbon nano tube. It is found that at low pressure, endohedral adsorption has higher hydrogen sulfide uptake against the exohedral, while at high perssure,exohedral adsorption exeeds the endohedral.This indicates that in applications of SWNTs for adsorption hydrogen sulfide gas at high pressure,exohedral adsorption or adsorption on outer surfaces of SWNTs might be significant and comparable with that inside the tubes.This suggestes that introduction of exohedral adsorption would improve adsorption at high pressures, while introduction of endohedral adsorption would improve adsorption at high temperature.

P(MP)	3	5	9	11
virial coefficients $(cm^3/molc)$	-248.7	-248.7	-248.7	-248.7
Number of gas molecules	540	5.95	1619	1979
In side density $(molecules/nm^3)$	7.40	5.95	4.15	5.01
Out side density $(molecules/nm^3)$	4.97	7.87	9.15	10.54
Total density $(molecules/nm^3)$	5.13	7.70	9.49	10.19

Table1-density of inside hydrogen sulfide adsorption on carbon nanotube,density of out side hydrogen sulfide on carbon nanotube, and density of total hydrogen sulfide adsorption

The shape of 1 show that relation between temperature and amount of hydrogen sulfide adsorption on carbon nanotube.

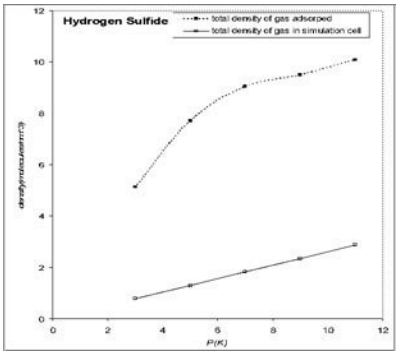

Figure 5. Relation between density of hydrogen sulfide gas and tempreture

Conclusion

The results show that the amount of adsorption increase with low temperature and high pressure. Now parents on how to use these nanotubes to remove toxic gas in Aluminium Industry.

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