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13. ABSTRACT (Maximum 200 words)

This report describes progress on a research project on using molecular modeling and simulation to understand the adsorption of water and other hydrogen bonded fluids in carbon materials. We describe progress on five research topics: i) We have developed a model for activated carbon adsorption. In this model the carbon is treated as a collection of randomly oriented platelets representing the graphene planes in carbon; ii) We have used this to study the adsorption of water in activated carbon. The model correctly describes behavior measured experimentally; iii) We have made a study of adsorption of water in slit shaped model pores to investigate the question of whether water can condense in pores without there being specific interactions with active sites; iv) As a first step in extending our work to the treatment of adsorption of mixtures of water and organic molecules in activated carbon we have made a study of mixtures of ethane and methane in activated carbon and compared our predictions with experiment; v) We have developed a lattice model for water adsorption in porous materials and have made calculations of water adsorption in carbon pores using this model.

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Modeling Adsorption of Hydrogen-Bonded Molecules in Porous Structures

Final Report

for the Period September 1, 2002 – November 30, 2004

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TABLE OF CONTENTS

Abstract

This report describes progress on a research project on using molecular modeling and simulation to understand the adsorption of water and other hydrogen bonded fluids in carbon materials. We describe progress on five research topics: i) We have developed a model for activated carbon adsorption. In this model the carbon is treated as a collection of randomly oriented platelets representing the graphene planes in carbon; ii) We have used this to study the adsorption of water in activated carbon. The model correctly describes behavior measured experimentally, including the temperature dependence of hysteresis loops; iii) We have made a study of adsorption of water in slit shaped model pores to investigate the question of whether water can condense in pores without there being specific interactions with active sites; iv) As a first step in extending our work to the treatment of adsorption of mixtures of water and organic molecules in activated carbon we have made a study of mixtures of ethane and methane in activated carbon and compared our predictions with experiment; v) We have developed a lattice model for water adsorption in porous materials. We have made Monte Carlo simulations of water adsorption in both a carbon slit pore and a coarse-grained activated carbon structure using this model.

1.0 INTRODUCTION

This final report describes research done on a project to investigate the fundamental mechanisms involved in the adsorption of water in carbon materials using molecular models. This project has its origin in the need for the development of filter materials that can be effective in high humidity environments. The design of new materials with low affinity for water that can maintain a high selectivity for other polar molecules would be of considerable interest in the design of advanced filters. A key component in the design of such materials is an understanding of how adsorption of water takes place at the microscopic level. Moreover, understanding the effects of strong association of other polar and hydrogen bonding organic molecules with active sites in carbon materials is also important. It is felt that the detailed molecular modeling of adsorption of associating fluids like water in different kinds of porous materials can contribute significant insight in this context. Our research group has developed extensive expertise in the molecular modeling of adsorption in porous materials. The current research program has exploited this expertise to tackle the problem of understanding water adsorption in porous materials.

In this report we describe progress on five research topics:

i) We have developed a model for activated carbon adsorption. In this model the carbon is treated as a collection of randomly oriented platelets representing the graphene planes in carbon;

ii) We have used this to study the adsorption of water in activated carbon. The model correctly describes behavior measured experimentally, including the temperature dependence of hysteresis loops;

iii) We have made a study of adsorption of water in slit shaped model pores to investigate the question of whether water can condense in pores without there being specific interactions with active sites;

iv) As a first step in extending our work to the treatment of adsorption of mixtures of water and organic molecules in activated carbon we have made a study of mixtures of ethane and methane and compared our predictions with experiment;

v) We have developed a lattice model for water adsorption in porous materials. We have made Monte Carlo simulations of water adsorption in both a carbon slit pore and a coarse-grained activated carbon structure using this model;

2.0 A MOLECULAR MODEL OF ADSORPTION IN ACTIVATED CARBON ADSORBENTS

Our model of activated carbon is an extension of one developed by Segarra and Glandt (1994). This model addresses the disorder in a porous carbon by treating the solid as a collection of platelets. The model is similar in spirit to a model of silica gel with which we have extensive experience (Kaminsky and Monson, 1991). A visualization of the model is shown in figure 1. Each platelet in the system models the effect of a single graphite basal plane (Segarra and Glandt used two basal planes in their model). The model provides a range of confinement environments. In some regions the confinement is similar to that in a slit pore. In others the graphite planes intersect at an angle. There is a significant spatial variation in the porosity and the model allows the possibility of collective effects beyond the length scale of a single pore. The parameters of our model are given in table 1.

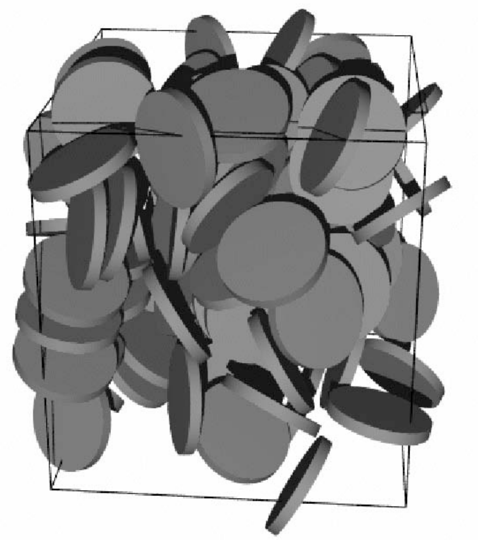

Figure 1. Platelet model of an activated carbon.

Table 1: Physical properties of the model carbon and of BPL carbon (estimated from experiments).

	Platelet Model	BPL Carbon
Diameter of platelet, nm	1.7	1.7 (Wolff, 1958)
Mass density, g/cm^3	0.88	0.872 (Sircar and Kumar, 1986)
Pore volume, cm^3/g	0.467 (4)	0.46-0.50 (Bradley and Rand, 1995)
Surface area, m^2/g	990 (47)	988-1120 (Reich et al., 1980; Barton et al., 1998; MacDonald et al., 2000; MacDonald and Evans, 2002)

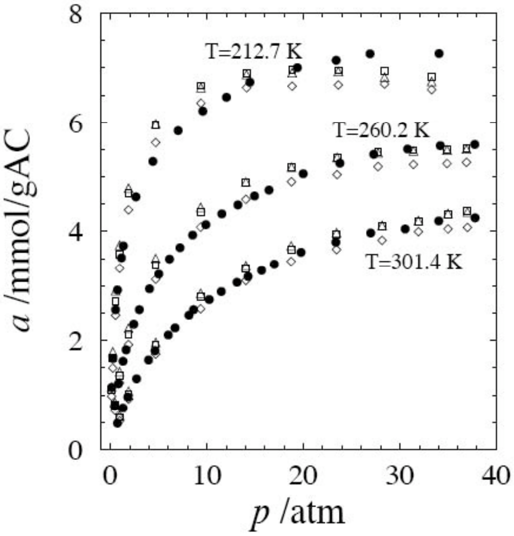

Figure 2. A comparison of adsorption isotherms from experiment (closed symbols) and Monte Carlo simulation (open symbols) for methane in activated carbon at three temperatures. Experimental data are from Reich et al. (1980).

The structural parameters for the carbon model were optimized by comparing the predictions from Monte Carlo simulations of methane adsorption with experimental results. This comparison is shown in figure 2. We have extended this calculation to ethane using a two-center Lennard-Jones potential to describe the ethane-ethane and ethane-carbon interactions and the other features of the carbon model were as used for the methane adsorption case. A comparison of our simulation results with experimental data at three temperatures is given in figure 3. The agreement is very good providing further support for the quality of the structural model.

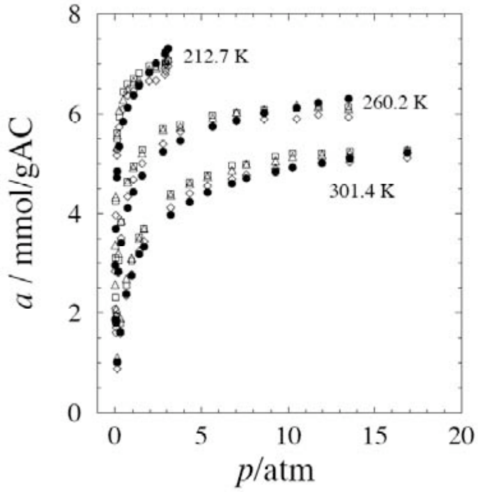

Figure 3. A comparison of adsorption isotherms from experiment (closed symbols) and Monte Carlo simulation (open symbols) for ethane in activated carbon at three temperatures. Experimental data are from Reich et al. (1980).

3.0 WATER ADSORPTION IN ACTIVATED CARBON

Using the model carbon presented in section 2 we have undertaken a study of water adsorption in activated carbon. In this case we have to include the short ranged directional interactions (hydrogen bonds) between the water molecules and for the water molecules with the active sites of the porous carbon. The approach we are taking is to include the effects of association primarily using nonelectrostatic potentials. This is motivated by our wish to have an intermolecular potential that it is sufficiently simple to allow a detailed study via Monte Carlo simulations together with a qualitatively realistic description of the hydrogen bonding. The basic idea is to add square well bonding sites to a spherically symmetric potential with the geometry chosen so that the number of association interactions saturates at a given value. This approach was originally developed for water by Nezbeda and coworkers (Kolafa and Nezbeda, 1987; Nezbeda et al., 1989, 1990, 1995) and models of this type are the basis of the Wertheim (1984a,b; 1987) statistical mechanical theory of associating fluids. They have been applied to adsorption of hydrogen bonded fluids in slit pores by Gubbins and coworkers (Müller and Gubbins, 1998) and by Sokolowski and coworkers (Huerta et al., 2000). In our work we model water as a Lennard-Jones 12-6 potential model with tetrahedrally coordinated square well sites. Throughout this report we will refer to this model as the LJ4SQW model.

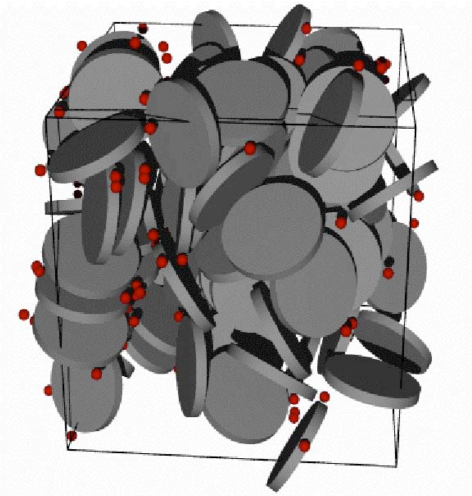

Figure 4. Visualization of platelet model of activated carbon with active sites. The red spheres are the active sites.

In order to model water adsorption we have to include a treatment of the association interaction of the water molecule with active sites of the carbon. For the effects of activation we add association sites in a random arrangement around the edge of the platelet. This is illustrated in figure 4. Figure 5 shows a visualization of water adsorbed in the model activated carbon from our Monte Carlo simulations. We note that the distribution of water in the porous material is highly inhomogeneous - water adsorption is mostly occurring around the edges of the platelets where it is easiest to develop the hydrogen bond network.

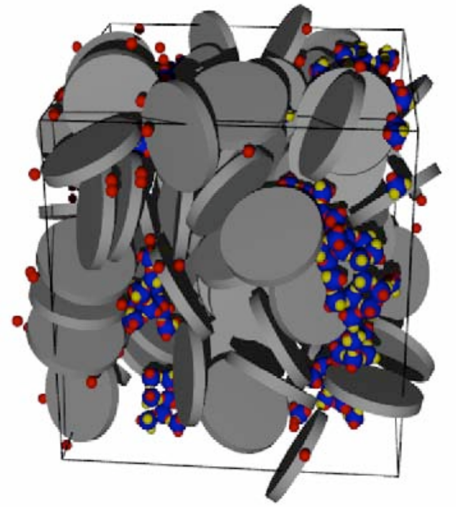

Figure 5. Visualization of water adsorption in platelet model with active sites.

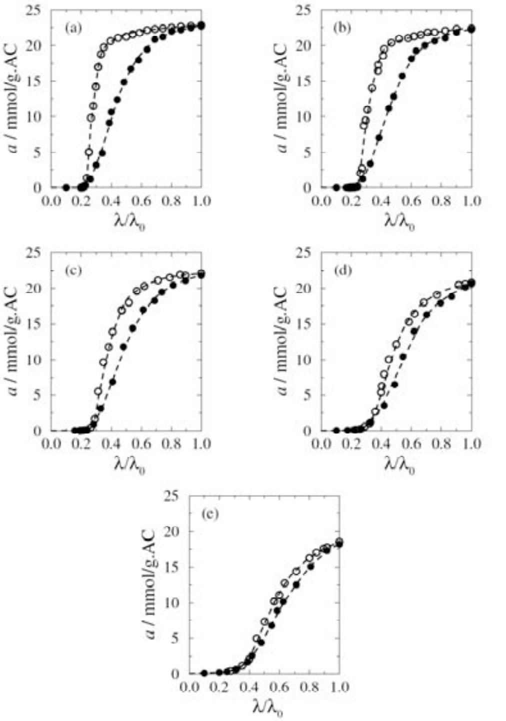

Figure 6. Sorption isotherms for LJ4SQW model of water adsorption in platelet model carbon for five temperatures a) 298.15K; b) 323,15K; c) 348.15K; d) 373.15K; e) 398.15K. Filled symbols for adsorption and open symbols for desorption. Lines are best fit to the simulation data, drawn as a guide to the eye.

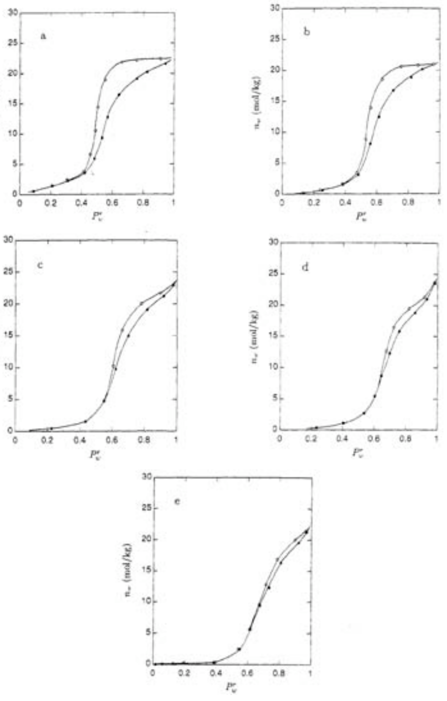

Figure 7. Sorption isotherms from experiment (Rudisill et al., 1992) of water adsorption in BPL carbon for five temperatures a) 298.15K; b) 323,15K; c) 348.15K; d) 373.15K; e) 398.15K. Filled symbols for adsorption and open symbols for desorption. Lines are best fit to the simulation data, drawn as a guide to the eye.

In order to test the validity of our model we have made calculations of the adsorption/desorption isotherms for water in activated carbon and compared the results with those from experiments. In particular we have focused our attention on the experiments carried out by Levan and coworkers (Rudisill et al., 1992) who have studied water adsorption in BPL carbon for a range of temperatures. Also for comparison we have made some calculations for a more complex model of water (the SPC model) that includes the electrostatic interactions. Figure 6 shows a set of isotherms calculated from the LJ4SQW model for five temperatures. We see that there is hysteresis in each case and that the width of the hysteresis decreases with increasing temperature. Figure 7 shows results from the work of Levan and coworkers. The quality of the agreement between the two is really quite impressive given the complexity of this problem. In particular we note the similarity in shape between the isotherms from the model and those from experiment. Figure 8 shows the corresponding results from the SPC model of water. The width of the hysteresis loops is somewhat narrower in this case but there is good qualitative agreement with the results from our model and from experiment.

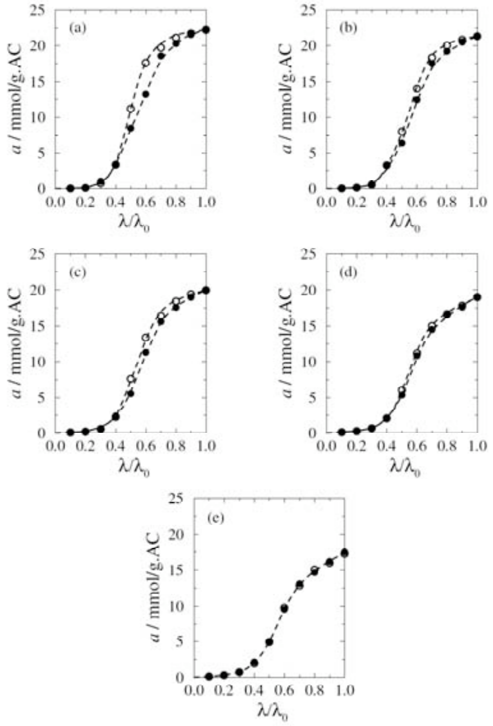

Figure 8. Sorption isotherms for SPC model of water adsorption in platelet model carbon for five temperatures a) 298.15K; b) 323,15K; c) 348.15K; d) 373.15K; e) 398.15K. Filled symbols for adsorption and open symbols for desorption. Lines are best fit to the simulation data, drawn as a guide to the eye.

4.0 DOES WATER CONDENSE IN CARBON PORES WITHOUT ACTIVE SITES ?

The traditional view of water adsorption in carbons is that unless there are active sites little adsorption takes at pressure below the vapor pressure of water. This is illustrated for example in figure 9, which shows experimental data for the adsorption of water on graphitized carbon black versus that of n-hexane. The stability of hydrogen bond network structures can be reduced by confinement in a porous material because the geometry of the confinement inconsistent with the network formation. Adsorbents in which only van der Waals type solid-fluid intermolecular forces occur should thus be hydrophobic. In our earliest results on the problem we found behavior consistent with this picture as shown in figures 10 and 11. Figure 10

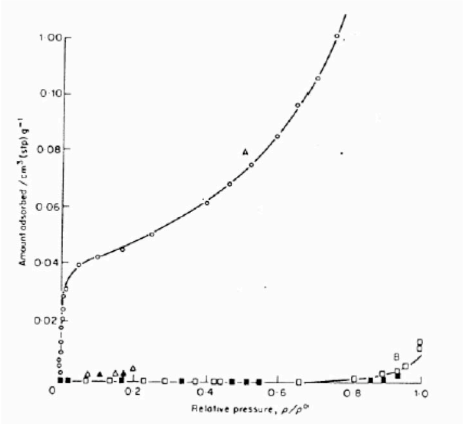

Figure 30: The adsorption isotherms of *n*-hexane (A) and of water (B) on graphitized carbon black. Filled symbols for desorption. (S.J. Gregg, K.S. Sing. Adsorption, Surface Area and Porosity. 2nd ed., Academic Press, New York, 1982.)

Figure 9. Adsorption isotherms for n-hexane (A) and water (B) on graphitized carbon black. (from S. J. Gregg and K. S. Sing, Adsorption Science and technology, Academic Press, new York, 1982).

shows results for methane in a carbon slit pore. We see that there is a hysteresis loop and that the pore fills with liquid for pressures less than the saturation pressure. Figure 11 has the corresponding results for the model of water we have been studying. This model treats the potential as a Lennard-Jones 12-6 potential together with tetrahedrally coordinated square well association sites. The latter interactions model the hydrogen bonds between the water molecules without the explicit inclusion of long ranged electrostatic interaction. Returning to figure 11 we see that here the adsorption remains very low until pressures much larger than the saturation pressure. The results in figures 10 and 11 are consistent with the notion of van der Waals pores being hydrophobic.

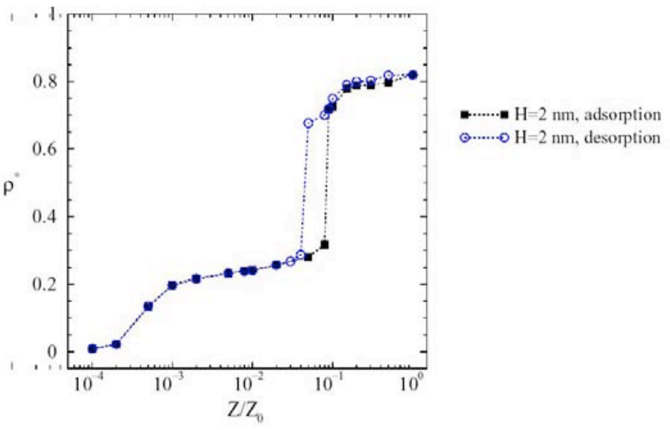

Figure 10. Adsorption/desorption isotherm for a model of methane in a slit pore. The x axis is the relative activity, which is equivalent to the relative pressure except for a small correction for gas imperfection.

In recent papers on simulation of water in slit pores (Striolo et al., 2003; Jorge and Seaton, 2003) an apparently different view is emerging. These researchers used the SPC and SPCE models of water interactions. These are more computationally intensive models and include electrostatic interactions associated with the

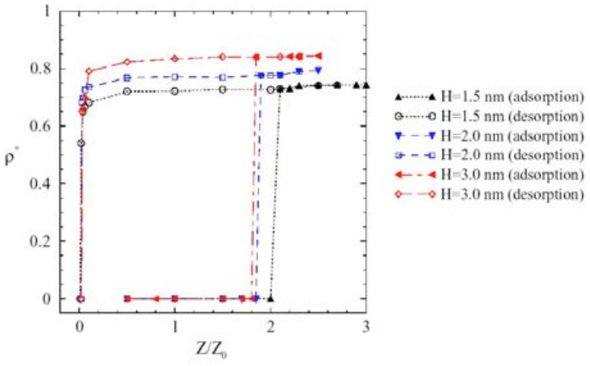

Figure 11. Adsorption/desorption isotherm for the LJ4SQW model of water in a slit pore for three values of the slit width H. The x axis is the relative activity, which is equivalent to the relative pressure except for a small correction for gas imperfection.

charge distribution in the water molecule. In both of these papers the results indicated that the water would condense in the pores at pressures below P_0. In a study like this it is important to establish a precise value of P_0 for the model. In the work of Striolo et al. (2003) they used a value of P_0 given by the pressure at which condensation occurs in a grand ensemble Monte Carlo simulation of the model in the bulk. This state is metastable and the pressure is much larger than the equilibrium vapor pressure. Jorge and Seaton (2003) used value of P_0 from an empirical equation of state. In both cases this leads to substantial overestimate of P_0 for the model. In view of the central importance to our project of understanding the nature of pore condensation for water we decided to examine the question in more detail.

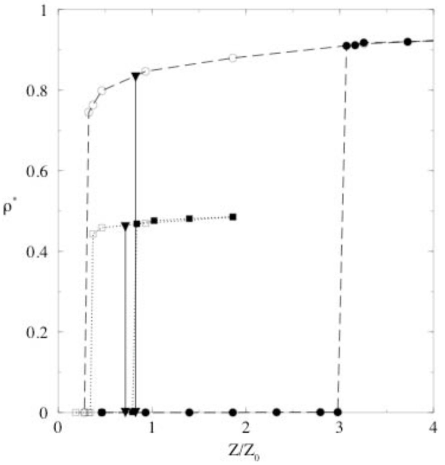

Figure 12. Adsorption/desorption isotherms for the SPC model of water in carbon slit pores for two different pore widths. Squares: 0.8 nm; Circles: 2.0 nm. The filled symbols denote adsorption and the open symbols denote desorption. The vertical solid lines denote the states where vapor-liquid equilibrium is predicted to occur in the pores. The x axis is the relative activity, which is equivalent to the relative pressure except for a small correction for gas imperfection.

We have made a study of this problem using three models of water: LJ4SQW, SPC/E, and SPC. The Steele 10-4-3 potential was used to calculate the fluid-wall interaction. We began by making a determination of the vapor pressure at 298K for each potential by using the Gibbs ensemble MC method to determine the vapor-liquid equilibrium state. We then determined the adsorption and desorption isotherms from GCMC simulations for the models for various pore widths and also the vapor-liquid equilibrium state for the confined water using the Gibbs ensemble method. As an example, our results for the SPC model of water are shown in figure 12 for several pore sizes. We found overall rough consistency between the behavior calculated for the LJ4SQW, SPC/E and SPC models. Water condenses in larger pores (>1 nm) at $P > P_0$. This behavior is consistent with what we had found in our earlier work on the LJ4SQW model and shown in figure 11. However, for narrower pores there may also be condensation for $P < P_0$. In the narrow pores the water molecules occupy a single layer in the slit and interact strongly with both pore walls. This interaction with both walls stabilizes the adsorbed water even though the environment for hydrogen bonding is unfavorable relative to the bulk liquid state. We have also calculated the vapor-liquid equilibrium for the water in the pores. In each case we find that this takes place at bulk pressures less than P_0. In real systems adsorption is generally accompanied by hysteresis so the point at which the condensation occurs in the pores is probably more relevant as a guide to whether water condenses in carbon pores than the phase equilibrium point.

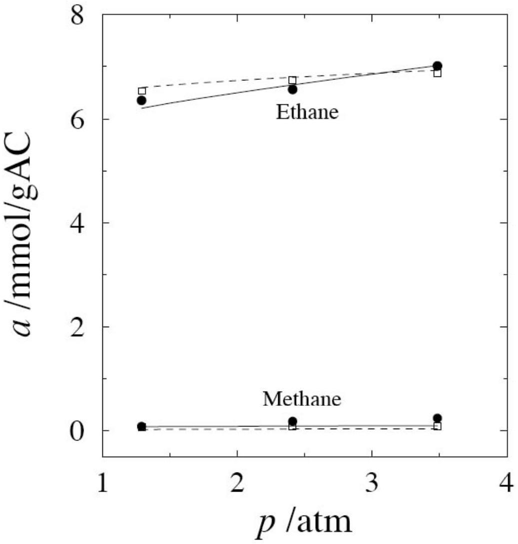

Figure 13. Component adsorption isotherms for 26.7% methane, 73.3% ethane mixtures in BPL carbon from Monte Carlo simulation, IAS theory, and experiment at T=212.7 K. Filled circles: experiment (Reich et al., 1980); Empty squares: MC simulation results for model carbon; Solid lines: IAS theory by using experimental pure component isotherms; Dash lines: IAS theory by using MC simulation pure component isotherms.

5.0 METHANE-ETHANE MIXTURES IN ACTIVATED CARBON

We have begun work on extending our project to mixtures. Ultimately our goal is to model mixtures of water and organic molecules, including polar organic molecules. Before doing this, however, it is important to test our methodology on simpler mixtures. We are focusing initially on mixtures of methane and ethane since this is a good base case for testing our simulation codes and the applicability of our model of carbon for mixtures. Figures 13 and 14 show a sample of our results at T = 212.7 K. Our simulation results are compared with experimental data (Reich et al., 1980) as well as the predictions of the ideal adsorbed solution (IAS) theory (Myers and Prausnitz, 1965). The ideal adsorbed solution theory gives an estimate of mixture adsorption from the pure component adsorption isotherms. We can apply two versions of this theory - one based on the experimental pure component isotherms and the other based on the pure component adsorption isotherms from the model. In our calculations we account for departures from ideal gas behavior in the bulk. Figure 13 shows the adsorption each component at three pressures and fixed temperature and figure 14 shows the adsorption of each component at several compositions for a fixed pressure and temperature. The agreement between all the calculations is very good showing that the molecular model is giving a good description of the experimental system and that the system is behaving as an ideal adsorbed solution.

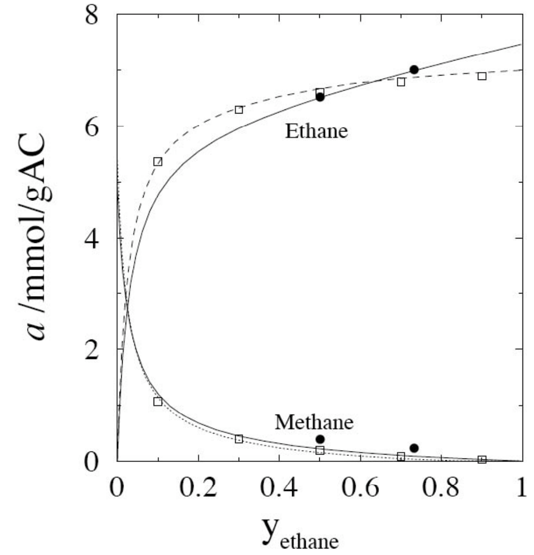

Figure 14. Component adsorption isotherms for methane-ethane mixtures in BPL carbon from Monte Carlo simulation, IAS theory, and experiment at T=212.7 K and P=3.40 atm. Legend is the same as for figure 13.

6.0 DEVELOPMENT OF A LATTICE MODEL OF WATER ADSORPTION IN CARBONS

The goal of this part of the work is to see if it is possible to develop a more economical approach to calculating the adsorption equilibrium in these systems that would still be based on molecular theory and would include the essential physics found in more complex models. In related projects on adsorption of molecules in complex pore structures we have developed a lattice model approach that has been very successful. Here we are extending this approach to the treatment of water adsorption.

The starting point of our work is a lattice model of water that includes the effect of orientation dependent association forces (Bell and Salt, 1976). This model uses a bcc lattice. The energy of a configuration involves three terms: i) an attractive interaction between nearest neighbor sites; ii) a hydrogen bonding interaction between nearest neighbor sites that depends only applies if the orientations of the molecules on those sites a aligned; iii) a repulsive interaction between next nearest neighbors on the lattice. The choice of bcc lattice is important since a bcc lattice can be used to represent two important ice phases: ice Ic which has a diamond structure similar to ice Ih and ice VII a high pressure phase with a bcc structure. The bcc lattice can be visualized as two interpenetrating diamond sublattices. Full occupation of one sublattice with orientational order corresponds to the ice 1c structure, while full occupation of both sublattices with orientational order corresponds to the ice VII structure. In addition the model can exhibit a low density gas-like phase and a liquid-like phase with a density intermediate between that of ice Ic and ice VII. Next nearest neighbor sites on a bcc lattice are always on different diamond sublattices. The repulsive next nearest neighbor interaction suppresses the simultaneous occupancy of both sublattices and thus provides stability for the ice Ic and liquid phases.

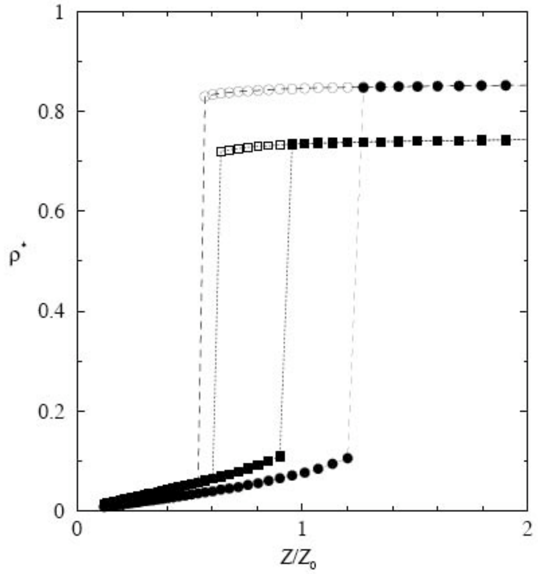

Figure 15. Adsorption desorption isotherms for the lattice model of water in a slit pore. The isotherms are for two different slite widths. Squares are for a pore of width 4 lattice units and the circles are for a pore of width 7 lattice units. The filled symbols denote adsorption and the open symbols denote desorption. The x axis is the relative activity which roughly equivalent to the relative pressure. For the narrow pore, the pore condensation takes place at pressures less than the bulk saturation pressure. For the wider pore the condensation takes place at pressures greater than the bulk saturation pressure.

We have recently carried out two sets of MC simulations for this model. In the first we have looked at adsorption of water in a slit pore using this model. Results for adsorption isotherms are shown in figure 15. The behavior observed is very similar to that described in section 4 of this report. The results are similar to that of off-lattice model as can be seen by comparing figure 15 with figure 11. Water condenses in larger pores at $P > P_0$ and water condenses in narrower pores for $P < P_0$. This similarity to off-lattice model indicates is encouraging and indicates that it will be worthwhile to use this lattice model for further investigations. We also performed GCMC simulations for lattice model water adsorption in a coarse graining of our modified platelet model. Preliminary results show a phenomenology very similar to that seen in the off-lattice model.

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