Equilibrium and Heat of Adsorption for Water Vapor and Activated Carbon

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ABSTRACT: The Qi-Hay-Rood adsorption isotherm equation is shown to provide an improved description of equilibrium water vapor adsorption onto microporous activated carbon between 298 and 373 K and total pressure at 101 kPa, when compared with an existing isotherm model. The influence of temperature on the isotherm equation's parameters is also quantified. An expression for the isosteric heat of adsorption is derived from the Clausius-Clapeyron equation. It is shown that the isosteric heat of adsorption decreases with increasing temperature and increasing adsorption capacity of water vapor. This new isotherm model can be inverted to describe water vapor concentration dependence on adsorption capacity and is therefore well suited for use in dynamic models for activated-carbon adsorption systems.

INTRODUCTION

Microporous activated-carbon adsorbents have been used extensively to remove a wide range of organic compounds from indoor air and industrial gas streams. Competitive adsorption between water vapor and organic compounds can reduce the adsorption capacities for the organic compounds, particularly at relative pressures (P/P_0, where P and P_0 = actual and saturated partial pressures of the adsorbate, respectively) of water vapor >0.6. Attrition and reduced adsorption capacities are often the determinants of service life of activated-carbon adsorbents. Therefore, it is important to understand and quantify the amount of water vapor adsorbed onto activated carbons and the competitive effects of water vapor on the adsorption of organic compounds. It is also important to quantify the isosteric heat of adsorption for water/activated-carbon systems. Such information can then be used to complete energy balances during the adsorption and desorption of water vapor when using activated carbon as the regenerable adsorbent.

Adsorption of water vapor onto activated carbon involves primary and secondary adsorptive sites (Dubinin 1980). Primary adsorptive sites consist of surface functional groups such as those that contain oxygen (Lizzio et al. 1990). These functional groups are capable of forming hydrogen bonds with water vapor. Secondary adsorptive sites consist of previously adsorbed water molecules. These adsorbed water molecules form hydrogen bonds with water vapor molecules as the water vapor approaches the surface of the activated carbon. Adsorption of water vapor occurs mainly on the primary adsorptive sites at low water vapor relative pressures. The number of available primary sites contributing to adsorption of water vapor decreases with increasing water vapor pressure as more water vapor adsorbs onto those sites. As water vapor pressure increases, adsorption occurs mainly on the secondary adsorptive sites of previously adsorbed water molecules. Equilibrium adsorption of water vapor onto microporous activated carbon is known to exhibit a Type-V isotherm according to the classi-

fication of Brunauer (Adamson 1976; Basmadjian 1997). Owing to this unique sigmoidal behavior caused by the primary and secondary adsorption sites, only a few adsorption isotherm models can be used to describe the adsorption of water vapor onto activated carbon. Models describing the equilibrium uptake of water vapor by activated carbon developed by Kisarov (1984), Mastroianni and Rochelle (1985), Dubinin and Serpinsky (1981), Barton et al. (1991), and Doong and Yang (1987) were reviewed by Huggahalli and Fair (1996). The review provides an overview of each model and describes why the Doong and Wang (DY) model is the most appropriate model available to describe the equilibrium uptake of water vapor by activated carbon. The DY model will be described and compared with the recently developed Qi, Hay, and Rood (QHR) model (Qi et al. 1998) in this paper. The Dubinin and Serpinsky (DS) model will also be described as it provides information needed for the DY model (Dubinin and Serpinsky 1981).

One commonly used isotherm model that describes adsorption of water vapor onto activated carbon is the DS model. The model is derived from consideration of dynamic equilibrium. The DS model is valid for P/P_0 values <0.6. A modification of the DS model by Barton et al. (1991) extended the DS model to describe the adsorption of water vapor over the entire range of P/P_0 values. This modified-DS model expresses adsorption capacity as a function of P/P_0 by an empirical four-parameter nonlinear equation. The equation is unsuitable for use in dynamic models describing the adsorption of water vapor onto activated carbon because it cannot be inverted to describe water vapor concentration dependence on equilibrium adsorption capacity (Huggahalli and Fair 1996).

Doong and Yang (1987) advanced the quantitative description of water vapor adsorption beyond the modified-DS model by including two additional parameters in the Dubinin-Radushkevich (DR) equation (Dubinin 1975). The DY model includes parameters to account for hysteresis h_0 and an activity coefficient γ to account for interactions between sorbates. The DY model has been used to describe the adsorption of water vapor onto BPL activated carbon from 298 to 373 K at 101 kPa total pressure by fitting the model to experimental data of Rudisill (1991). These graphical results were obtained from Huggahalli and Fair (1996) and presented in Fig. 1.

Qi et al. (1998) developed the QHR isotherm model to describe adsorption of water vapor onto activated carbon. The model recognizes that adsorption capacity of water vapor changes due to changes in the number of available primary and secondary adsorptive sites with increasing water vapor pressure (Dubinin 1980). The sigmoidal shape of the adsorption isotherm results from the change in available types of adsorptive sites with increasing water vapor pressure. The QHR isotherm model was verified using experimental data for water vapor adsorption onto four different activated carbon

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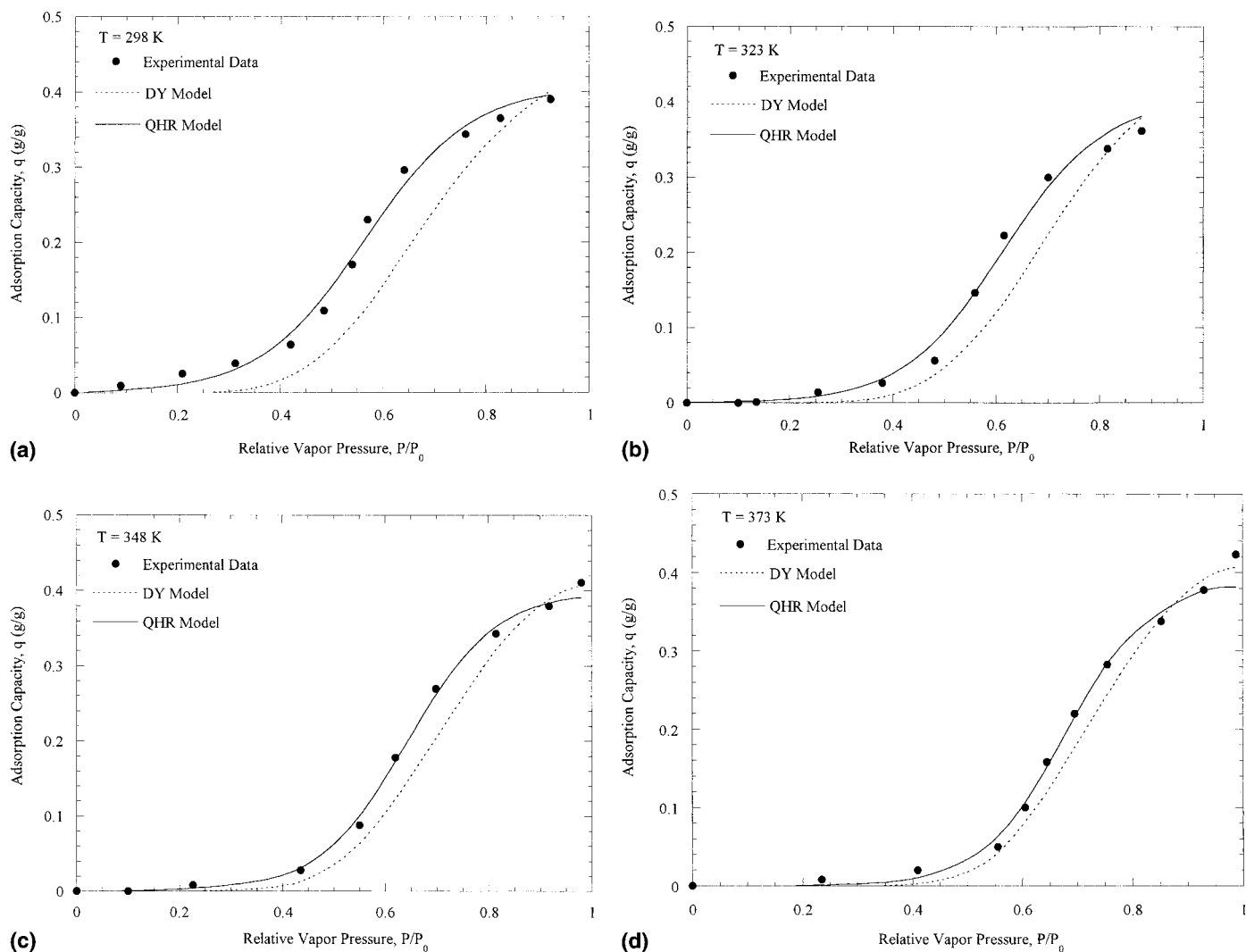
FIG. 1. Comparison of Experimental Data (Rudisill 1991) to Results from DY Model (Huggahalli and Fair 1996) and Results from QHR Model (Qi et al. 1998) at: (a) 298 K; (b) 323 K; (c) 348 K; (d) 373 K

adsorbents from 288 to 308 K at 101 kPa total pressure (Qi et al. 1998). The model is also suitable for use in dynamic models describing the adsorption of water vapor onto activated carbon because it can be inverted to describe equilibrium water vapor concentration dependence on equilibrium adsorption capacity.

In this paper, the QHR model is presented, compared, and contrasted with the DY model. The effect of temperature on the QHR isotherm parameters is also quantified. An expression for the isosteric heat of water vapor adsorption onto activated carbon is then derived from the classic Clausius-Clapeyron equation.

ISOTHERM MODELS

The DS model is given as

$$q = (k_1)(q + q')(1 - k_2 q)\left(\frac{P}{P_0}\right) \qquad (1)$$

where q = adsorption capacity of water; and k_1, q', and k_2 = fitted parameters determined from the water vapor adsorption data at P/P_0 values <0.6. An alternative to (1) used by Huggahalli and Fair (1996) is a two-parameter correlation developed by Dubinin (1980) and modified by Pacheco (1995). The resulting equation is easier to use but is limited to P/P_0 values <0.6. Reliable characterization of water vapor adsorption onto activated carbon at P/P_0 values >0.6 are of particular impor-

tance with respect to competitive adsorption between organic compounds and water vapor for air quality engineering related applications (Cal et al. 1996).

The DY model is written with consideration of the density of adsorbed water ρ as follows (Doong and Yang 1987):

$$q = \rho V_0 \exp\left\{-\left(\frac{T}{\beta E}\right)^2 \left(\ln \frac{\gamma P_0}{P}\right)^2 - (\ln h_0)^2\right\} \qquad (2)$$

where q = adsorption capacity of water vapor; ρ = density of adsorbed water; V_0 = limiting pore volume of the absorbent; T = absolute temperature; β and E are DR isotherm parameters (Dubinin 1975); γ = coefficient to account for different degrees of association in the liquid and adsorbed phases; P/P_0 = relative pressure of the water vapor; and h_0 accounts for hysteresis. The value for h_0 is set equal to P/P_0 at the beginning of the hysteresis loop. The value of γ is determined empirically and is dependent on P/P_0. The value for $\gamma(P/P_0 < 0.6)$ is calculated using the DS equation, whereas $\gamma(P/P_0 > 0.6) = 1$ (Doong and Yang 1987).

The QHR isotherm model for adsorption of water vapor by microporous activated carbon is as follows:

$$q = \frac{\rho V_0}{1 + \exp\left[k\left(\frac{P_{1/2}}{P_0} - \frac{P}{P_0}\right)\right]} \qquad (3)$$

where q, ρ, and V_0 are described above. The terms $P_{1/2}$ and k

are empirically derived constants obtained by fitting the experimental data to the model (Qi et al. 1998). Therefore, V_0, $P_{1/2}$, and k are experimentally derived values obtained by fitting the experimentally derived adsorption isotherm to the model. The QHR model does not consider hysteresis as described by the DY model.

COMPARISON OF MODELED TO EXPERIMENTAL RESULTS

The QHR and DY models are compared and contrasted by presenting results from both models when using experimental adsorption isotherm results from Rudisill (1991). Results for the DS model are not considered here because the DY and QHR models are applicable for P/P_0 values $\lesssim 0.95$, whereas the DS model is limited to P/P_0 values <0.6. As previously stated, P/P_0 values >0.6 are very important for air quality engineering related applications. The experimental isotherm data describe water vapor adsorption onto BPL activated carbon (Calgon Carbon Corp., Pittsburgh, Pa.) at 101 kPa total pressure and from 298 to 373 K (Fig. 1). Characterization of a different sample of BPL activated carbon using N_2 adsorption isotherm data and a 3D model resulted in a total pore volume of 0.58 cm^3/g with 88% of those pores existing in the microporous region. Average micropore size of the BPL activated carbon was 8.8 Å and its average overall pore size was 13.9 Å (Sun 1999). This total pore volume is larger than the pore volume obtained with data from Ruddisil (1991) of 0.35 cm^3/g or from Hassan et al. (1991) of 0.41 cm^3/g indicating varying properties of the BPL activated carbon and differences in methods to determine the activated carbon's properties. Such results indicate why it is important to use the same data set from the same lot of activated carbon when comparing modeled with experimental results. Results from the DY model describing adsorption of water vapor onto BPL activated carbon were obtained from Huggahalli and Fair (1996) as presented in Fig. 1. The DY model systematically underpredicts the experimentally determined equilibrium adsorption capacity data. Agreement between the experimental and modeled results is described using the mean absolute percent difference of q as follows:

Mean Absolute Percent Difference in

$$q_i = \left(\frac{100}{N}\right) \sum_{i=1}^{N} \left| \frac{q_{i,\text{measured}} - q_{i,\text{modeled}}}{q_{i,\text{measured}}} \right| \qquad (4)$$

where N = number of P/P_0 values used to determine the corresponding values for q; $q_{i,\text{measured}}$ = measured adsorption capacity; and $q_{i,\text{modeled}}$ = modeled adsorption capacity using the DY or QHR models. Mean absolute percent differences for the DY model decrease from 52.7 to 13.3% as temperature increases from 298 to 373 K (Table 1). Mean absolute percent differences for the QHR model decrease from 19.1% to 4.6% as temperature increases from 298 K to 373 K (Table 1). Best-

fit isotherm parameters for the QHR model are provided in Table 1. The parameters were determined with a nonlinear least-squares optimization program written in FORTRAN that includes a subroutine from the International Mathematical and Statistical Libraries (*Visual* 1994).

Limiting pore volume V_0 of the BPL adsorbent was determined when the values for $P_{1/2}/P_0$ and k were quantified at the reference condition of 298 K and 101 kPa [Fig. 1(a)]. The resulting value for V_0 was then kept constant, as a structural property of the adsorbent, when values for $P_{1/2}/P_0$ and k were determined at 323, 348, and 373 K [Fig. 1(b–d), respectively]. Limiting pore volume was previously shown to be constant, as a structural property of the adsorbent, for BPL activated carbon between 288 and 308 K, and it was linearly related to the N_2-BET specific surface area (Qi et al. 1998). The corresponding values of V_0 for three different microporous activated-carbon fiber-cloth adsorbents using adsorption of water vapor and adsorption of organic vapors such as acetone, benzene, and toluene were shown to be within a relative difference of $<10\%$ (Foster et al. 1992, Qi et al. 1998). Such results indicate that V_0 can be treated as a constant structural property of the adsorbent, and the thermal expansion of activated-carbon adsorbent has a negligible effect on V_0 for this temperature range.

The parameter $P_{1/2}/P_0$ for BPL activated carbon increases by 20.4% as temperature increases from 298 to 373 K. The dependence of $P_{1/2}/P_0$ on T is well described by a linear regression

$$\frac{P_{1/2}}{P_0} = a + bT \qquad (5)$$

where $a = 0.121$; $b = 1.50 \times 10^{-3}$ K^{-1}. The linear regression coefficient R^2 for (5) is 0.996.

Parameter k for BPL activated carbon increases 38.7% as temperature increases from 298 to 373 K. The following Arrhenius-type equation is used to approximate the dependence of k on T:

$$k = Ae^{-(E_a/RT)} \qquad (6)$$

where $A = 51.96$; and $E_a = 4.105$ kJ/mol. The regression coefficient R^2 for (6) is 0.981.

Eqs. (5) and (6) may be substituted into (3) to obtain an expression for the Type-V isotherm that explicitly includes the effect of temperature on the equilibrium relationship between q and P/P_0.

ISOSTERIC HEAT OF ADSORPTION

The isosteric heat of adsorption at constant adsorption capacity Q_q can be determined using the Clausius-Clapeyron equation (Hersh 1961; Talu and Kabel 1987)

$$Q_q = -R \left(\frac{\partial \ln(P)}{\partial(1/T)} \right)_q = R \frac{T^2}{P} \left(\frac{\partial P}{\partial T} \right)_q \qquad (7)$$

TABLE 1. Mean Absolute Errors for DY and QHR Models and Resulting Adsorption Isotherm Parameters for QHR Model When Using BPL Activated Carbon and Water Vapor at 1 atm

Temperature (K) (1)	Mean absolute error for DY model (%) (2)	Mean absolute error for QHR model (%) (3)	V_0 (cm^3/g) (4)	$P_{1/2}/P_0$ (5)	k (6)
298	52.7	19.1	0.407	0.564	10.17
323	25.6	9.0	0.407	0.612	10.82
348	23.1	3.5	0.407	0.642	12.47
373	13.3	4.6	0.407	0.679	14.11
Arithmetic mean absolute errors	28.7	9.0	—[a]	—[a]	—[a]
Standard deviation of absolute errors	16.9	7.1	—[a]	—[a]	—[a]

[a]Not applicable.

The expression for P is obtained from the inversion of (3)

$$P = P_0 \left(\frac{P_{1/2}}{P_0} - \frac{1}{k} \ln \left(-\frac{V_0\rho - q}{q} \right) \right) \qquad (8)$$

Assuming V_0 is independent of temperature, differentiating (8) at constant q gives

$$\left(\frac{\partial P}{\partial T} \right)_q = \frac{P}{P_0} \frac{dP_0}{dT} + P_0 \frac{d}{dT} \left(\frac{P_{1/2}}{P_0} \right) + \frac{P_0}{k^2} \ln \left(\frac{V_0\rho - q}{q} \right) \frac{dk}{dT}$$

$$+ \frac{P_0 V_0}{k} \left(\frac{q}{V_0\rho - q} \right) \frac{d\rho}{dT} \qquad (9)$$

Eqs. (7) and (9) suggest that Q_q varies with both temperature and adsorption capacity. The four derivatives in (9) are evaluated analytically below.

Saturated vapor pressure of water P_0 can be described by the Wagner equation (Reid et al. 1987)

$$P_0 = P_c \exp \left(\frac{a_1 x + a_2 x^{1.5} + a_3 x^3 + a_4 x^6}{1 - x} \right) \qquad (10)$$

where $x = (1 - T/T_c)$; T_c = critical temperature; P_c = critical pressure; and $a_1 - a_4$ = constants that are specific for water vapor. Differentiating (10) gives

$$\frac{dP_0}{dT} = \frac{P_0}{T_c} \left(\frac{-a_1 - 1.5a_2 x^{0.5} + 0.5a_2 x^{1.5} - 3a_3 x^2 + 2a_3 x^3 - 6a_4 x^5 + 5a_4 x^6}{(1 - x)^2} \right) \qquad (11)$$

The density of adsorbed water ρ in the pores of the adsorbent is assumed to be equal to the bulk liquid density of water at temperatures below water's normal boiling point at 101 kPa total pressure. For temperatures above the normal boiling point, an adjustment similar to the one made by Dubinin (1975) may be necessary. For temperatures up to 100°C at 101 kPa, ρ is modeled using data from Dean (1992)

TABLE 2. Values for Parameters in Eq. (11) Describing Density of Liquid Water

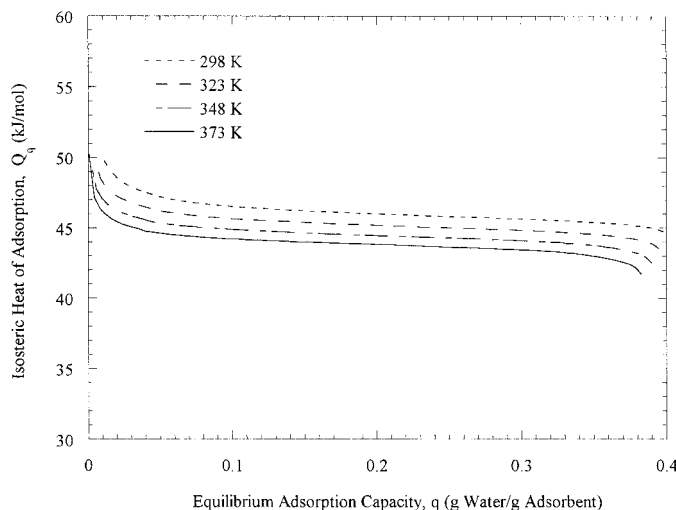| b_0 (kg/m³) (1)	b_1 (kg/m³/°C) (2)	b_2 (kg/m³/°C²) (3)	b_3 (kg/m³/°C³) (4)	b_4 (kg/m³/°C⁴) (5)
999.87	5.3809×10^{-2}	-7.6924×10^{-3}	7.4783×10^{-5}	-1.4733×10^{-7}

FIG. 2. Isosteric Heats of Adsorption of Water Vapor on BPL Activated Carbon and Its Dependence on Temperature and Amount of Adsorbed Water

by regressing the data with a fourth-order polynomial equation

$$\rho = b_0 + b_1 t + b_2 t^2 + b_3 t^3 + b_4 t^4 \qquad (12)$$

where $t = T - 273.15°C$; and $b_0 - b_4$ = fitted constants (Table 2). The regression coefficient R^2 of (12) is 1.000. Differentiating (12) yields

$$\frac{d\rho}{dt} = b_1 + 2b_2 t + 3b_3 t^2 + 4b_4 t^3 \qquad (13)$$

Differentiating (5) gives

$$\frac{d}{dT} \left(\frac{P_{1/2}}{P_0} \right) = b \qquad (14)$$

Differentiating (6) gives

$$\frac{dk}{dT} = A \frac{E_a}{RT^2} \exp \left(-\frac{E_a}{RT} \right) = \frac{E_a k}{RT^2} \qquad (15)$$

Eqs. (9), (11), and (13)–(15) are then substituted into (7) to determine Q_q. Values for Q_q are shown to decrease with increasing T and q as described in Fig. 2. These results are now available for use with energy and material balances when modeling the adsorption cycle of the water vapor/activated-carbon adsorbent system. The calculated value for Q_q at 373 K approaches 41.23 kJ/mol as P/P_0 approaches unity. This value of Q_q is within 1.4% of the heat of condensation for bulk water, 40.66 kJ/mol (Dean 1992), for water vapor at its normal boiling point with total pressure = 101 kPa.

SUMMARY AND CONCLUSIONS

A new isotherm model, referred to as the QHR model, is shown to be in better agreement with experimental water vapor adsorption data than the existing DY model for a predominantly microporous coal-based activated carbon from 298 to 373 K and a total pressure of 101 kPa. The QHR model contains three isotherm parameters, limiting pore volume V_0, k, and $P_{1/2}/P_0$. The limiting pore volume V_0, a structural parameter for the adsorbent, was kept constant; $P_{1/2}/P_0$ increases linearly by 20.4%; and k increases by 38.7% following the Arrhenius equation, as temperature increases from 298 to 373 K. The isosteric heat of adsorption for water vapor is shown to decrease with increasing temperature and adsorption capacity. The isosteric heat of adsorption is within 1.4% of the heat of condensation for water vapor as relative pressure approaches unity. The QHR isotherm model can also be inverted to describe water vapor concentration dependence on adsorption capacity and is thus well suited for use in dynamic models describing the adsorption of water vapor by microporous activated-carbon adsorption systems.

APPENDIX I. REFERENCES

Adamson, A. W. (1976). *Physical chemistry of surfaces*, 3rd Ed., Wiley, New York.

Barton, S. S., Evans, M. J. B., and MacDonald, J. A. F. (1991). "The adsorption of water vapor by porous carbon." *Carbon*, 29, 1099.

Basmadjian, D. (1997). *The little adsorption book. A practical guide for engineers and scientists.* CRC, Boca Raton, Fla.

Cal, M., Rood, M. J., and Larson, S. M. (1996). "Removal of VOCs from humidified gas streams using activated carbon cloth." *Gas. Sep. Purif.*, 10(2), 117–121.

Dean, J. A. (1992). *Lange's handbook of chemistry*, 14th Ed., McGraw-Hill, New York.

Doong, S. J., and Yang, R. T. (1987). "Adsorption of mixtures of water vapor and hydrocarbons by activated carbon beds: Thermodynamic model for adsorption equilibrium and adsorber dynamics." *Recent progress in adsorption and ion exchange*, Y. H. Ma and J. P. Ausikaitis, eds., *AIChE, Symp. Ser. No. 259*, 83, 87–97.

Dubinin, M. M. (1975). ''Physical adsorption of gases and vapors in micropores.'' *Progress in surface and membrane science*, D. A. Cadenhead, J. E. Danielli, and M. D. Rosenberg, eds., Vol. 9, Academic, New York.

Dubinin, M. M. (1980). ''Water vapor adsorption and the microporous structure of carbonaceous adsorbent.'' *Carbon*, 18, 355.

Dubinin, M. M., and Serpinsky, V. V. (1981). ''Isotherm equation for water vapor adsorption by microporous carbonaceous adsorbents.'' *Carbon*, 19, 402.

Foster, K. L., Fuerman, R. G., Economy, J., Larson, S. M., and Rood, M. J. (1992). ''Adsorption characteristics of trace organic compounds in gas streams onto activated carbon fibers.'' *Chem. Mat.*, 4, 1068–1073.

Hassan, H. M., Ghosh, T. K., Hines, A. L., and Loyalka, S. K. (1991). ''Adsorption of water vapor onto BPL activated carbon.'' *Carbon*, 29(4/5), 681–683.

Hersh, C. K. (1961). *Molecular sieves*. Reinhold, New York.

Huggahalli, M., and Fair, J. R. (1996). ''Prediction of equilibrium adsorption of water onto activated carbon.'' *Ind. Engrg. Chem. Res.*, 35, 2071.

Kisarov, M. M. (1984). ''Isotherm equation for the adsorption of water vapor on carbon adsorbents.'' *Zh. Fiz. Khim.*, 58, 1980–1983.

Lizzio, A., Jiang, H., and Radovic, L. (1990). ''On the kinetics of carbon (char) gasification: Reconciling models with experiments.'' *Carbon*, 28(1), 7–19.

Mastroianni, M. L., and Rochelle, S. G. (1985). ''Improvements in acetone adsorption efficiency.'' *Envir. Prog.*, 4, 7–13.

Pacheco, M. A. (1995). ''Modeling and simulation of co-adsorption of water vapor and organic compounds in fixed-bed activated carbon beds,'' MS thesis, University of Texas at Austin, Austin, Tex.

Qi, S., Hay, K. J., and Rood, M. J. (1998). ''Isotherm equation for water vapor adsorption onto activated carbon.'' *J. Envir. Engrg.*, ASCE, 124(11), 1130–1134.

Reid, R. C., Prausnitz, J. M., and Poling, B. E. (1987). *The properties of gases and liquids,* 4th Ed., McGraw-Hill, New York.

Rudisill, E. N. (1991). ''Studies on water-hydrocarbon adsorption equilibria and adsorptive and membrane separations,'' PhD dissertation, University of Virginia, Charlottesville, Va.

Sun, J. (1999). ''Preparation, evaluation and structural modeling of carbon-based adsorbents on natural gas vehicles,'' PhD dissertation, University of Illinois, Urbana-Champaign, Ill.

Talu, O., and Kabel, R. L. (1987). ''Isosteric heat of adsorption and the vacancy solution model.'' *AIChE J.*, 33(3), 510–514.

Visual numerics. (1994). *FORTRAN subroutines for mathematical applications, Vol. 2*, Houston, International Mathematical and Statistical Libraries (IMSL).

APPENDIX II.   NOTATION

The following symbols are used in this paper:

A, E_a = regression constants in Eq. (6);

a = regression constants in Eq. (5);

a_1, a_2, a_3, a_4 = constants in Eq. (10) for saturated water vapor pressure;

b = regression constants in Eq. (5) (K^{-1});

b_0, b_1, b_2, b_3, b_4 = regression constants in Eq. (12) for liquid water density;

E = DR isotherm parameter (energy constant) in Eq. (2) (T^2);

h_0 = constant to account for hysteresis in Eq. (2);

k = QHR isotherm constant in Eq. (3);

k_1, k_2, q' = DS isotherm parameters in Eq. (1);

Q_q = isosteric heat of adsorption at constant loading;

q = equilibrium adsorption capacity of water at P;

q_0 = maximum adsorption capacity;

P = vapor pressure of water;

P_c = critical vapor pressure of water;

P_0 = saturation vapor pressure of water;

$P_{1/2}$ = isotherm constant and $P = P_{1/2}$ at $q/q_0 = 1/2$;

T = temperature (K);

T_c = critical temperature of water (K);

t = temperature (°C);

V_0 = limiting pore volume;

x = $(1 - T/T_c)$;

β = DR isotherm parameter (affinity coefficient) in Eq. (2);

γ = coefficient to accounting for degrees of association in liquid and adsorbed phases; and

ρ = density of adsorbed water.