
Virtual Group Theory - A New Method to Calculate the Adsorption Equilibrium of Organic Mixtures for Respirator Protection Applications

Frank Ding and M. Douglas LeVan

Department of Chemical and Biomolecular Engineering, Vanderbilt University,
Nashville, TN 37235, U.S.A
E-mail: YDING@TYCOINT.COM

ABSTRACT

A new method, virtual group theory or VGT, is developed to predict multi-component adsorption equilibrium of organic vapors, and hence the service life time of filter cartridges. The method is developed based on the theory that adsorbed organic contaminants can be treated as a virtual liquid mixture, while the adsorption effect is taken as a virtual group that dilutes the mixture, hence reducing the saturated vapor pressure of each component. The resulting virtual vapor-liquid equilibrium is then solved by traditional group contribution models such as the UNIFAC model. Test calculations for a number of organic vapors have demonstrated that the VGT method can accurately predict adsorption equilibrium of organic vapors and their mixtures. Also, the VGT can predict adsorption equilibrium of the organic mixtures at different humidity levels.

Keywords: adsorption, equilibrium, group contribution

INTRODUCTION

The service life of a respiratory protection organic vapor (OV) cartridge is dependent largely on the adsorption equilibrium of specific contaminants under given site conditions. In most practices, such adsorption equilibrium is calculated using empirical correlation models. One widely used adsorption equilibrium model in the respiratory protection industry is the D-R equation. Wood has correlated a number of breakthrough data of single organic vapor on carbon-based adsorbents, and developed prediction model that correlates the adsorption potential model parameters in the D-R equation to the molar polarization value of the contaminant chemical (Wood 1994, 1987ab, 2001, 2004, 2005, 2007). While this approach can provide reasonable prediction for certain organic vapor adsorption equilibrium on activated carbon, it may result in more deviation if the organic chemical contains some special functional groups, especially those with hydrophilic properties or those with special chemical adsorption properties. One other effort of the direct calculation of the adsorption equilibrium of mixtures was started by Myers and Pausnitz (1965) with the Adsorbed Solution Theory (AST). In this theory, they assume that the adsorption equilibrium of a gas mixture can be expressed as an equilibrium between the gas phase and an adsorbed phase by equating the fugacity in the two phases. LeVan and coworkers (Appel et al., 1998, Taqvi and LeVan, 1997) have used a Virial-type description for the activity coefficients of binary mixtures.

In this research, we proposed a different approach in predicting adsorption equilibrium, namely the *Virtual Group Theory* (VGT). This approach is based on the group contribution theory that has been

successfully used in the prediction of *Vapor Liquid Equilibrium* (VLE), which is based on the theory that a physical or chemical property of a chemical is a sum of the attributions of all constituent functional groups. The VGT model as we described below applies to both pure component adsorption equilibrium and the adsorption equilibrium of mixtures, including mixtures of OV and water.

THEORY

The fundamental assumption of the virtual group theory is that vapor-adsorbate adsorption equilibrium can be solved following vapor-liquid equilibrium by assuming that the adsorption potential is equivalent to virtual diluents. With such an assumption, an adsorption equilibrium problem can be solved using a traditional group contribution method in much the same way that a vapor-liquid equilibrium problem is solved. In this case, the virtual diluents are represented by the presence of virtual groups. Consequently, one can write adsorption equilibrium as

$$P_i = \Gamma_i X_i P_i^s \quad (1)$$

where P_i is the equilibrium vapor pressure of an adsorbate at a given adsorption loading, X_i is the molar fraction of the adsorbate in the virtual mixture, P_i^s is the saturated vapor pressure of adsorbate i in liquid state, and Γ_i is the activity coefficient that is calculated using traditional group contribution models.

One of the group contribution models that has been successfully used in VLE prediction is the UNIFAC model (Fredenslund *et al.*, 1975; Fredenslund *et al.*, 1977; Fu *et al.* 1996; Lohmann *et al.*, 2001; Poling *et al.*, 2001; Gmehling *et al.*, 2002). In the UNIFAC model, the activity coefficient Γ_i is expressed as the sum of two parts:

$$\ln \Gamma_i = \ln \Gamma_i^c + \ln \Gamma_i^r \quad (2)$$

where Γ_i^c is the combinatorial part expressed by

$$\ln \Gamma_i^c = \ln \frac{\Phi_i}{X_i} + \frac{z}{2} s_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{X_i} \sum_j X_j l_j \quad (3)$$

$$l_i = 5(r_i - s_i) - (r_i - 1)$$

while Γ_i^r is the residual part expressed by

$$\ln \Gamma_i^r = \sum_k (v_k \ln \Gamma_k - \ln \Gamma_k^{(i)}) \quad (4)$$

$$\ln \Gamma_k = S_k \left(1 - \ln \sum_m (\Theta_m \Psi_{mk}) - \sum_m \frac{\Theta_m \Psi_{mk}}{\sum_n (\Theta_n \Psi_{nm})} \right) \quad (5)$$

$$\Theta_m = \frac{S_m X_{gm}}{\sum_n (S_n X_{gn})} \quad (6)$$

$$\Psi_{mn} = \exp \left(-\frac{A_{mn}}{T} \right) \quad (7)$$

Here the parameters r_i and s_i respectively represent the van der Waals volume and the van der Waals surface area of a component, which are calculated from the contributions of each individual groups using

$$r_i = \sum_k \nu_k R_k \quad (8)$$

$$s_i = \sum_k \nu_k S_k \quad (9)$$

Note in the above UNIFAC equations, there are three parameters to be determined for each group: R , S , and A_{mn} . The parameters S and R are normalized group parameters representing the surface area and volume of the group. The parameter A_{mn} is the normalized group interaction energy parameter. For common functional groups listed in the literature, the values of these parameters have been calculated or correlated by previous researchers and are readily available (e.g., Poling *et al.*, 2001). Thus, in order to solve the virtual VLE problem derived from the VGT, the remaining parameters are the values of R , S , A_{mn} , and the molar density of the virtual group at a given adsorption filling fraction. The values of R and S can be estimated from the atomic size of the adsorbent surface. For activated carbon, the values of R and S are estimated as $R = 0.8165$ and $S = 0.8744$, taking the virtual group size the same as that of carbon atoms, of which the diameter is 0.34 nm (Horvath and Kawazoe, 1983).

Two parameters must be correlated from experimental adsorption equilibrium data for each individual group on a specific sorbent material. These are the group interaction parameter for the virtual group to the real group (noted as A_{vr}) and the virtual group molar density at a given filling fraction (noted as n_v).

METHODS

In order to use the proposed VGT to predict adsorption equilibrium, the parameter A_{vr} for every constituent functional group must be correlated from experimental data. Also, a curve of virtual group density versus the filling fraction has to be obtained using an adsorption isotherm of a probe chemical. Below is a typical procedure

- Step 1. Create a curve of virtual group density versus the filling fraction using an adsorption isotherm data of a probe chemical.
- Step 2. Estimate the values of S and P for the virtual group for the target adsorbent. For activated carbon, these values are estimated as 0.82 and 0.87, respectively.
- Step 3. Correlate the A_{vr} value of the functional groups of interest from the experimental adsorption equilibrium data of simple chemicals. If humidity is involved in the prediction, correlate the A_{vr} value of the group H_2O from the experimental adsorption equilibrium data of water. (Note that the use of simple chemicals in the correlation process can avoid the use of toxic chemicals, the adsorption equilibrium of which may be of primary interest in predicting by the group contribution method.)
- Step 4. Using the UNIFAC equations, predict the adsorption equilibrium of any chemical mixture (including water) of which the constituent functional groups are in the list of Step 3. Note that the vapor pressure data or model parameters must be available for all of the chemicals, as these are needed for the calculation.

For convenient practical applications, we suggest that a small database of A_{vr} be collected for common functional groups for a particular adsorbent of interest. With this database, the adsorption equilibrium of the organic chemicals and their mixtures can be predicted.

To collect the database of A_{vr} values for the functional groups, one should start with simple chemicals that consist of a single type of group. For example, a simple alkane (e.g., hexane) shall be used here to obtain the A_{vr} of the group CH_x . Here $x = 0$ to 4 denotes any number of hydrogen atoms bonded to the group. Pure water adsorption equilibrium data, as a special instance, shall be used to correlate the A_{vr} for the functional group of H_2O .

For the functional groups that do not exist alone in a chemical molecule, simple chemicals that contain only this group and one or more types of group of which the A_{vr} values have already been collected. For instance, the adsorption equilibrium data of ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) (consisting of two CH_x groups and one OH group), can be used to collect the A_{vr} value of the group OH, provided that the A_{vr} value for CH_x has been collected *á priori*.

Note that with the VGT method, the adsorption equilibrium of mixtures is calculated the same way as that of single chemicals - no special rules are needed. This applies to mixtures with water, provided that the A_{vr} value for water is correlated. To obtain the values of A_{vr} for the target groups, we fit the entire isotherms for the chemical. We find that best-fit value of A_{vr} has a dependency to the isotherm temperature. Thus, we also fit the A_{vr} to the temperature by using the linear relation

$$A_{vr} = \alpha_v + \beta_v(T - 298.15) \quad (10)$$

SAMPLE PREDICTIONS

To demonstrate the VGT method, we have chosen some simple, non-toxic or low toxicity chemicals as our candidates. Although these chemicals are typically of less importance in the respiratory protection industry due to their low toxicities, they can still provide good examples for the prediction of adsorption equilibrium using the VGT method.

These chemicals are classified into two groups: group one is for correlating VGT parameters, while group two is used for verifying the adsorption equilibrium prediction. The adsorption equilibrium data for all of these chemicals have been obtained by previous researchers and are published on the literature. Tables I and II list the chemicals in the two groups. Note that not all the group parameters we collected in Group 1 correlation are used in Group 2 prediction.

Table I. List of Group 1 Chemicals for Correlating VGT Parameters

Chemical	Molecular Structure	Constituent Groups	Target Group
Water	H_2O	H_2O	H_2O
n-Hexane	$\text{CH}_3(\text{CH}_2)_4\text{CH}_3$	CH_x	CH_x
Ethanol	$\text{CH}_3\text{CH}_2\text{OH}$	CH_x ; OH	OH
Acetone	CH_3HCO	CH_xCO	CH_xCO
Dimethylether	CH_3OCH_3	CH_x ; OCH_x	OCH_x
Dichloromethane	CH_2Cl_2	CH_2Cl_2	CH_2Cl_2

Table II. List of Group 2 Chemicals and Chemical Mixtures for Test Prediction

Chemical / Mixtures	Molecular Structure	Constituent Groups
Ethane	CH_3CH_3	CH_x
Octane	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$	CH_x
Butanol	$\text{CH}_3(\text{CH}_2)_3\text{OH}$	CH_x ; OH
MTBE	$(\text{CH}_3)_3\text{COCH}_3$	CH_x ; OCH_x
Octane-Hexane	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$; $\text{CH}_3(\text{CH}_2)_4\text{CH}_3$	CH_x
Ethane-Water	CH_3CH_3 ; H_2O	CH_x ; H_2O

The adsorbent we use in this research is the BPL activated carbon produced by Calgon Carbon Corporation USA. To obtain the virtual group density curve, we used the adsorption isotherms of propane on the BPL carbon at 25 °C. In this research, we use the saturated liquid density as proposed by Spence and Danner (1972) to approximate the density of the adsorbed phase.

Figures 1 through 6 show the fitting results for these chemicals. We plot the water adsorption isotherms on a linear scale rather than the semi-log scale we used for the rest of the figures, because we want to show that the VGT can fit the distinctive S-shaped curve of the water adsorption isotherm. Note that these are fittings of the experimental data in order to obtain the values of A_{vr} , but not actual predictions. The results show that the model can fit to the experimental data well for the various chemicals. Thus, a small database of A_{vr} (in the form of α_v and β_v) is obtained (see Table 3) for the target functional groups. From Table 3 we find that the VGT parameters are closely related to the polarity of the group: more polar groups tend to have more positive group interaction energy (as revealed in the values of α_v). Meanwhile, the interaction energy values for more polar groups are more sensitive to temperature changes (as revealed by the values of β_v).

Note that for the purpose of theoretical research, we simulate the concentrations over a wide range up to the condensation point (shown as the vertical portion of the curves). Also we cover a very wide range of isotherm temperatures. In respiratory protection industry, the applicable concentration and temperature ranges are typically much narrower.

Table III. List of the VGT Parameters Correlated from the Experimental Data

Group	α_v, K	β_v
CH_x	-579.7	1.57
OH	196.4	12.89
H_2O	429.5	5.99
CH_xCO	-333.0	2.91
OCH_x	-417.3	0.93
CH_xCl_2	-531.3	1.99

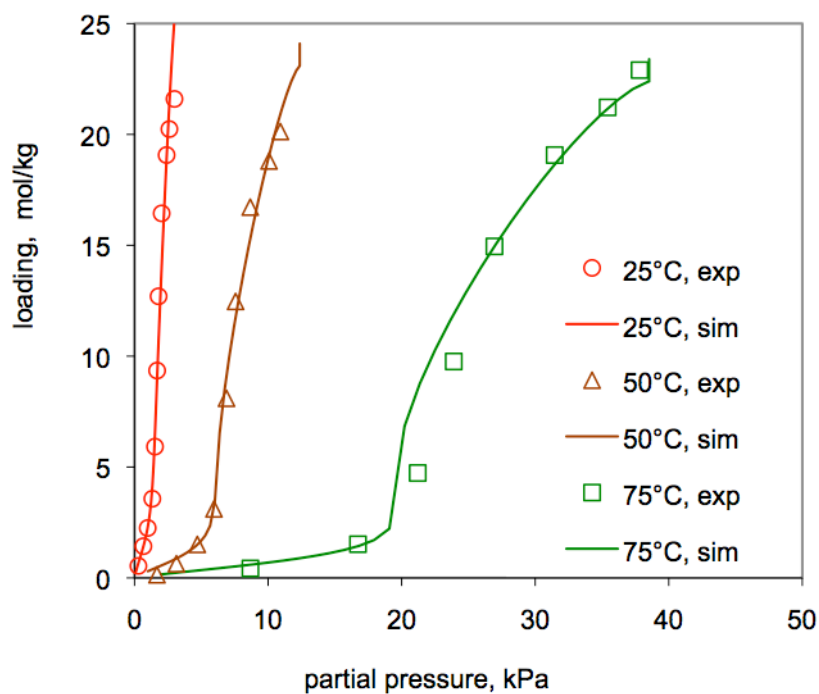


Figure 1. VGT correlation of water adsorption isotherms on BPL carbon (experimental data: Rudisill *et al.*, 1992).

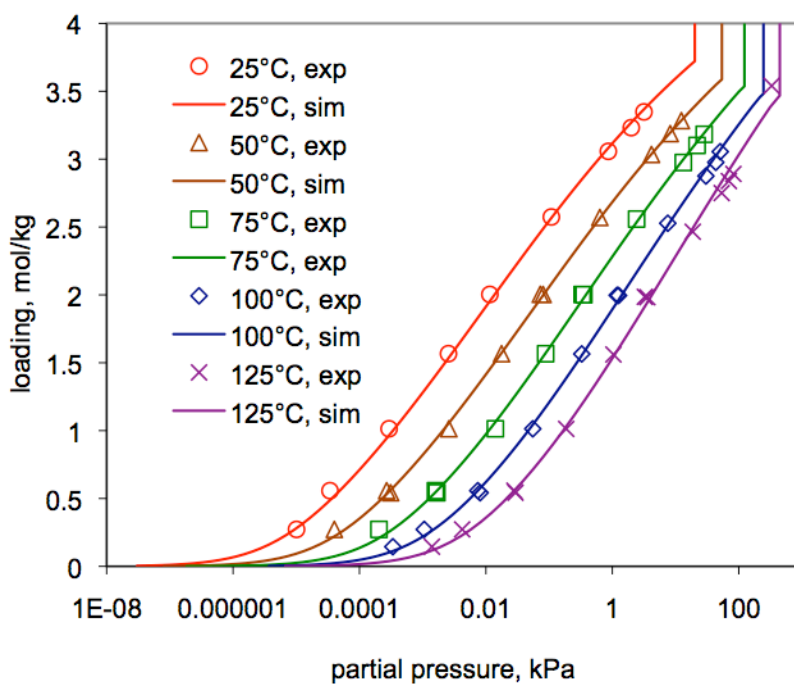


Figure 2. VGT correlation of n-hexane adsorption isotherms on BPL carbon (experimental data: Rudisill *et al.*, 1992).

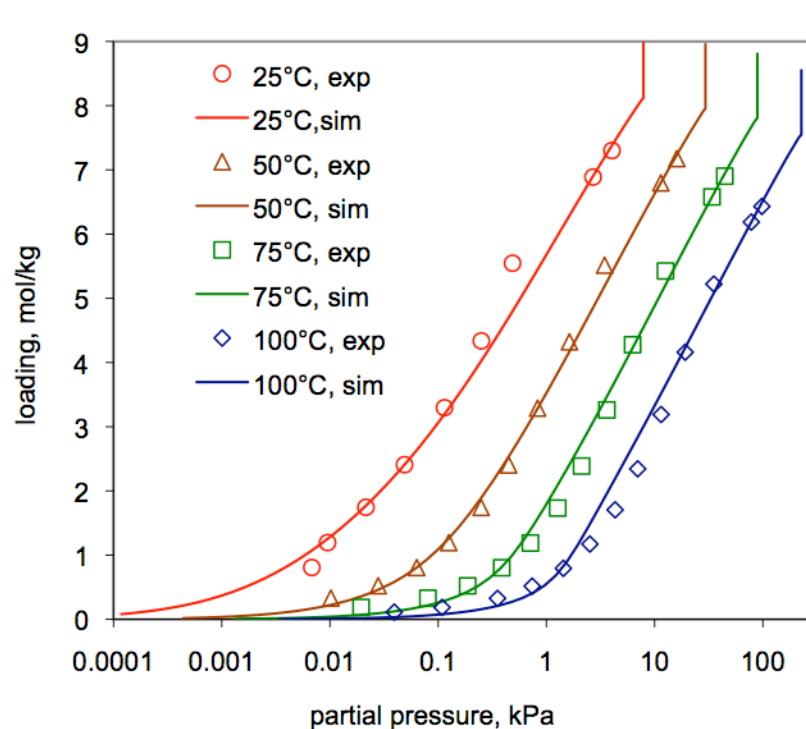


Figure 3. VGT correlation of ethanol adsorption isotherms on BPL carbon (experimental data: Taqvi *et al.*, 1999).

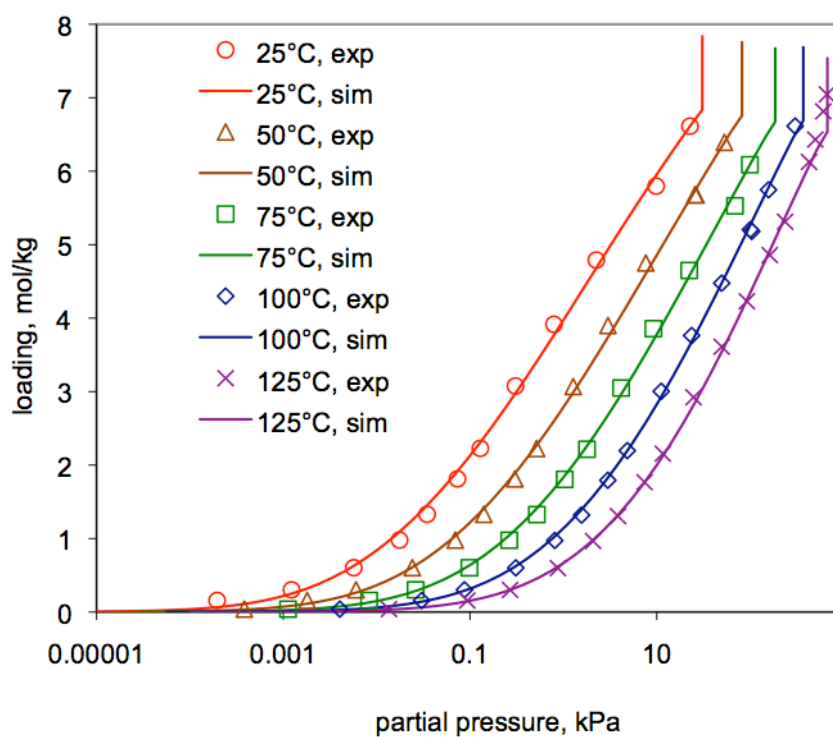


Figure 4. VGT correlation of acetone adsorption isotherms on BPL carbon (experimental data: Rudisill *et al.*, 1992).

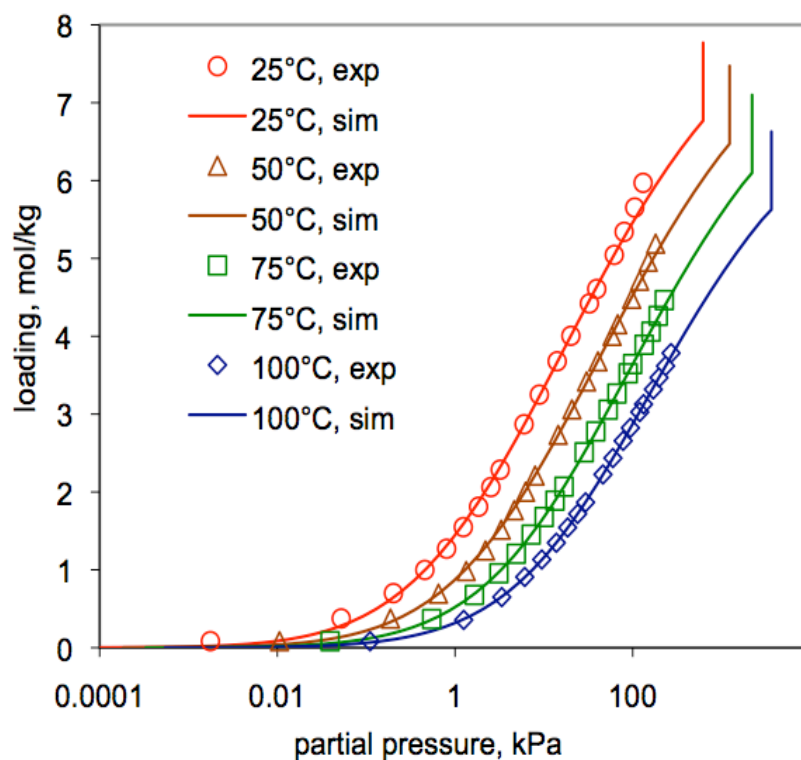


Figure 5. VGT correlation of dimethylether adsorption isotherms on BPL carbon (experimental data: Ding, 2002).

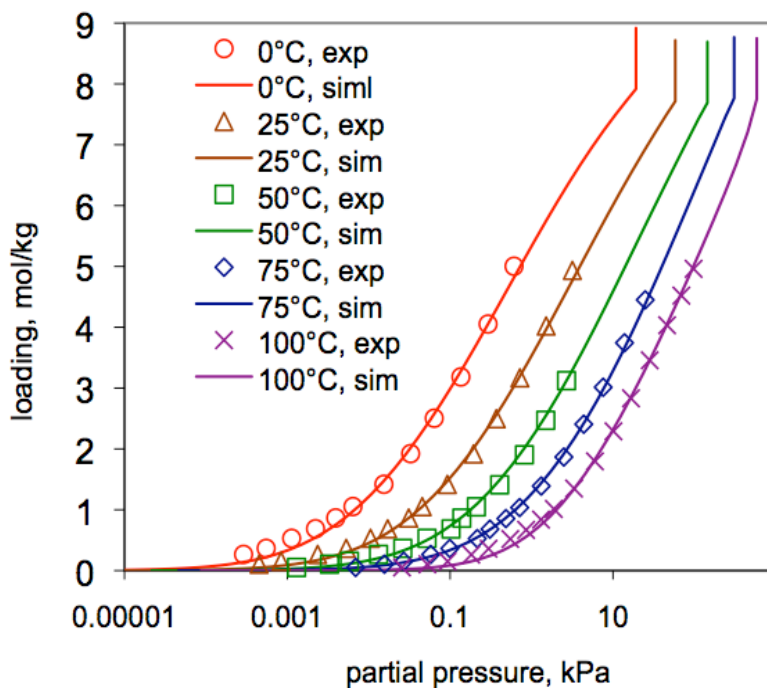


Figure 6. VGT correlation of dichloromethane adsorption isotherms on BPL carbon (experimental data: Eissmann and LeVan, 1993).

Using the A_{vr} values obtained, we can now predict the adsorption equilibrium for the chemicals and chemical mixtures listed in Table II. Figures 7 through 12 show the predicted adsorption equilibrium (shown in the figures as the solid lines of adsorption isotherms) in comparison with the experimental data (shown in individual data points). Note in Figure 12 water loading is not present as the data were not collected by the authors (Russell and LeVan, 1997). From these figures we see that satisfactory prediction accuracy is achieved for most of the data points. The prediction accuracy is slightly lower if the molecular structure is somewhat complicated, such as the ones containing both hydrophobic groups and hydrophilic groups, such as butanol. This is reasonable due to the fact that when groups of a largely different nature are mixed together their interactions are harder to simulate. Nevertheless, the prediction results are still satisfactory.

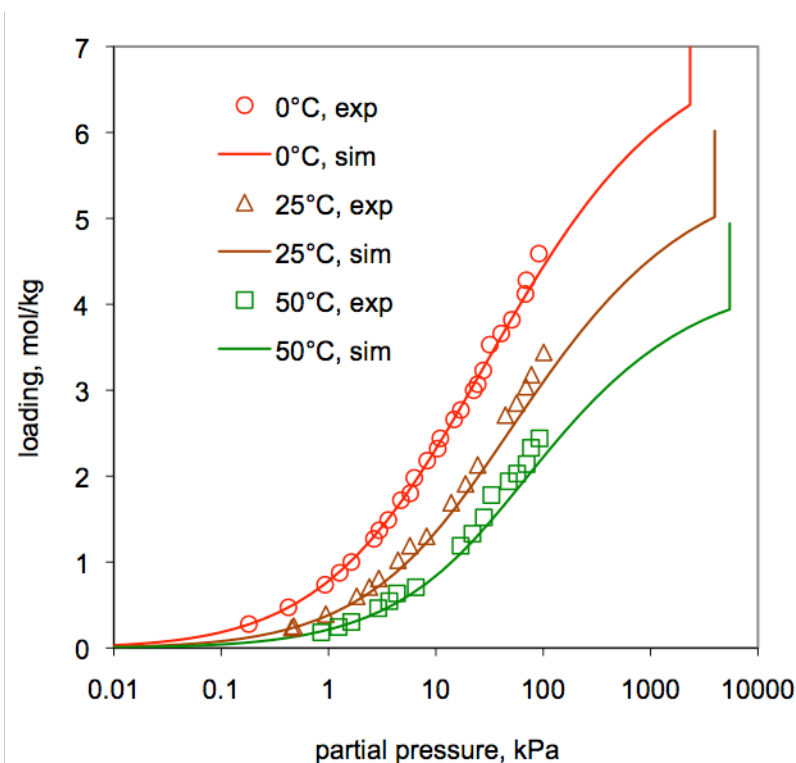


Figure 7. VGT prediction of ethane adsorption isotherms on BPL carbon (experimental data: Russell and LeVan, 1997).

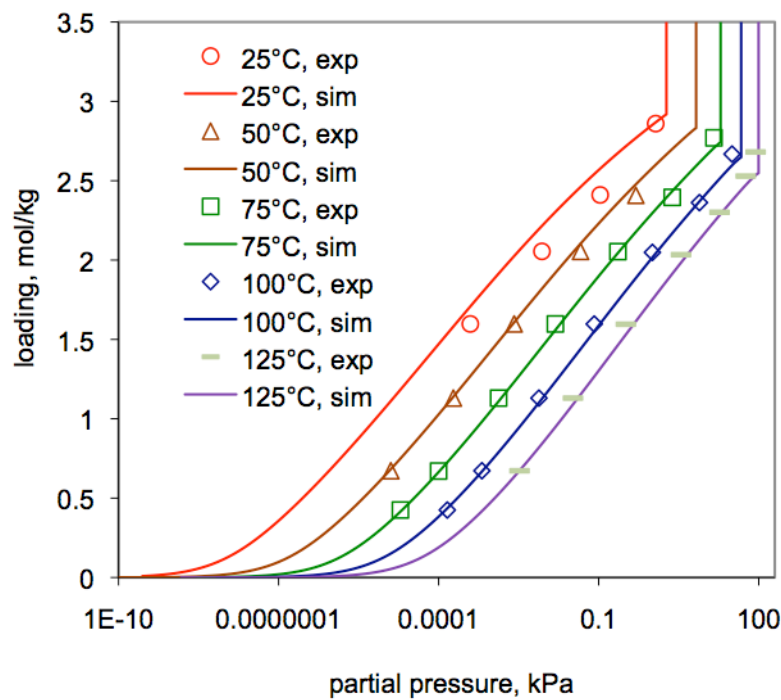


Figure 8. VGT prediction of octane adsorption isotherms on BPL carbon (experimental data: Hacskeylo, 1987).

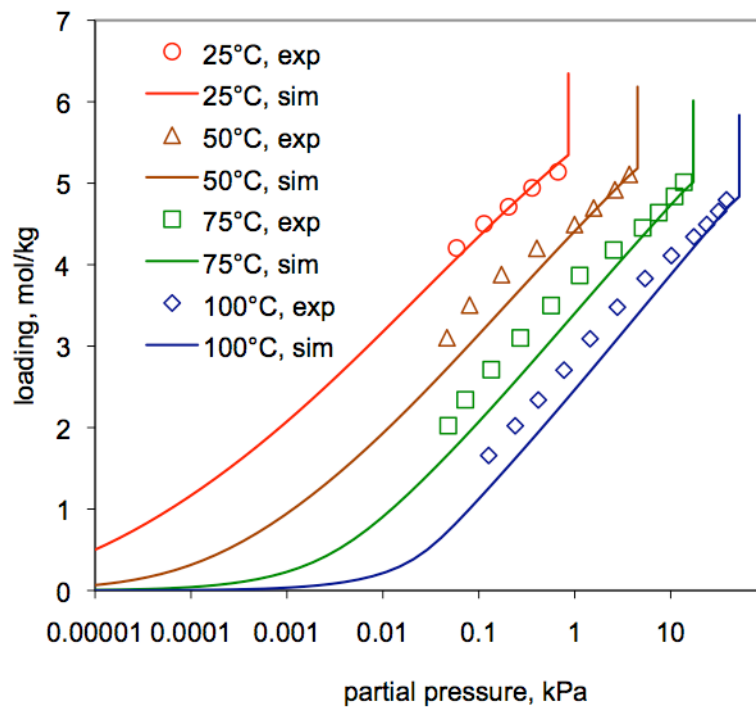


Figure 9. VGT prediction of butanol adsorption isotherms on BPL carbon (experimental data: Taqvi et al., 1999).

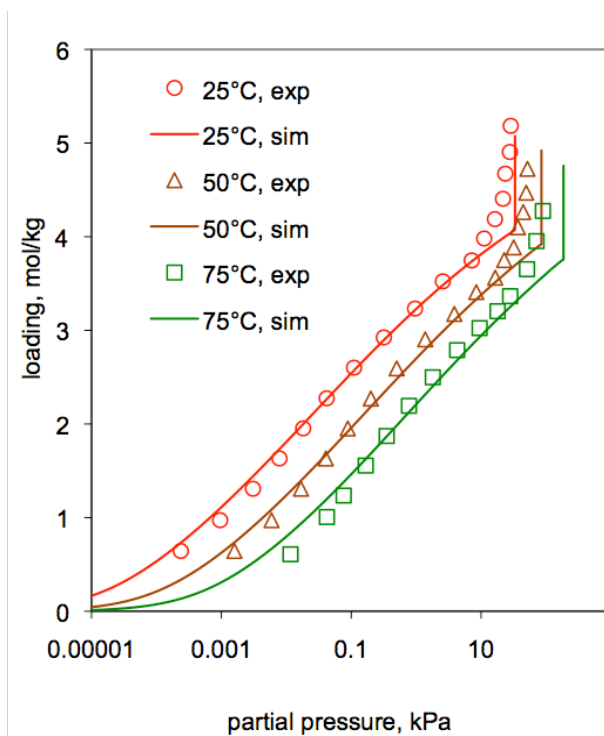


Figure 10. VGT prediction of MTBE adsorption isotherms on BPL carbon (experimental data: Ding, 2002).

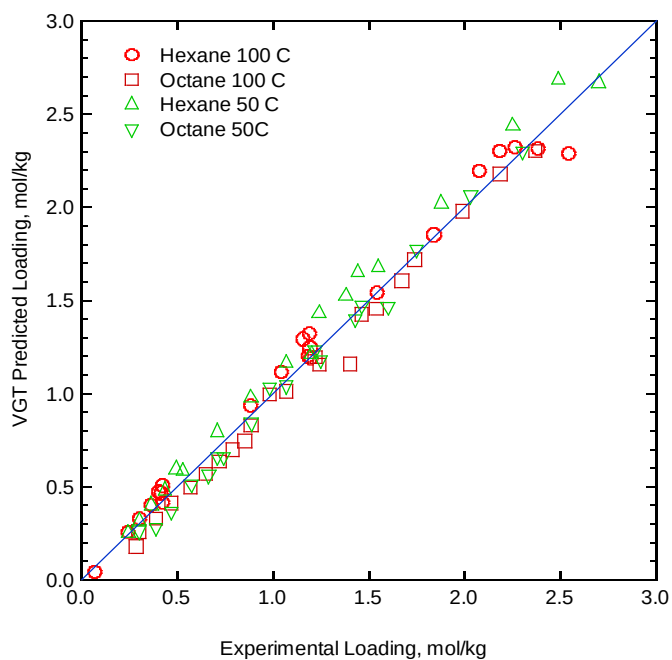


Figure 11. VGT prediction of the adsorption equilibrium of octane-hexane mixtures on BPL carbon (experimental data: HacsKaylo, 1987).

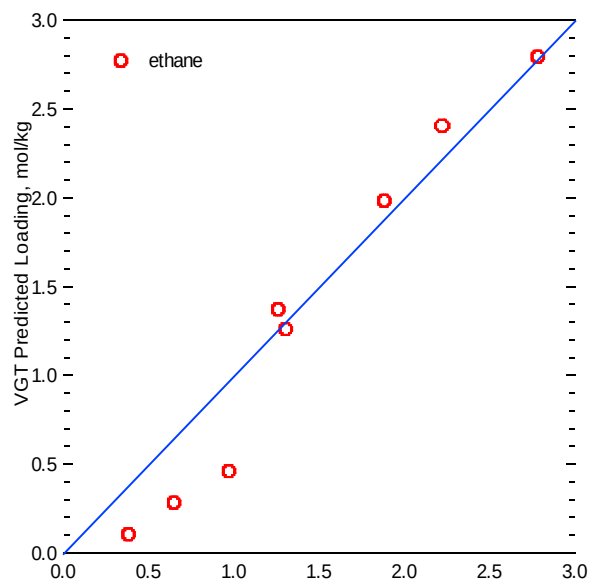


Figure 12. VGT prediction of the adsorption equilibrium of ethane-water mixtures on BPL carbon. (experimental data: Russell and LeVan, 1997).

Note that for the two mixtures, it is inconvenient to show the 3-dimensional equilibrium data. Thus, as an alternative, we plot the predicted adsorption loading values versus the measured loading values so the prediction accuracy can be compared. Figures 13 and 14 show the prediction results. Each curve represents a fixed adsorption loading value for the chemical. We see that for the hexane-octane mixture, the curves for the hexane loading and the octane loading cross each other to a large extent, meaning that these two chemicals can co-exist to some extent. On the contrary, the curves for ethane loading and water loading can no longer cross each other very much, indicating that the two chemicals have a strong tendency to repel each other and can hardly co-exist. This is coincident with the common recognition that chemicals with the similar polarity tend to co-adsorb better than chemicals with different polarity.

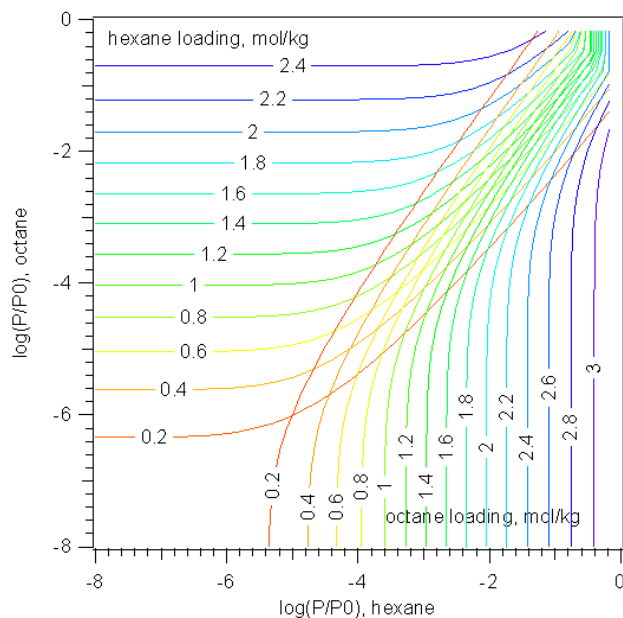


Figure 13. VGT prediction of the adsorption equilibrium of octane-hexane mixtures on BPL carbon. Each line represents a fixed loading for octane (top-left) and hexane (bottom-right).

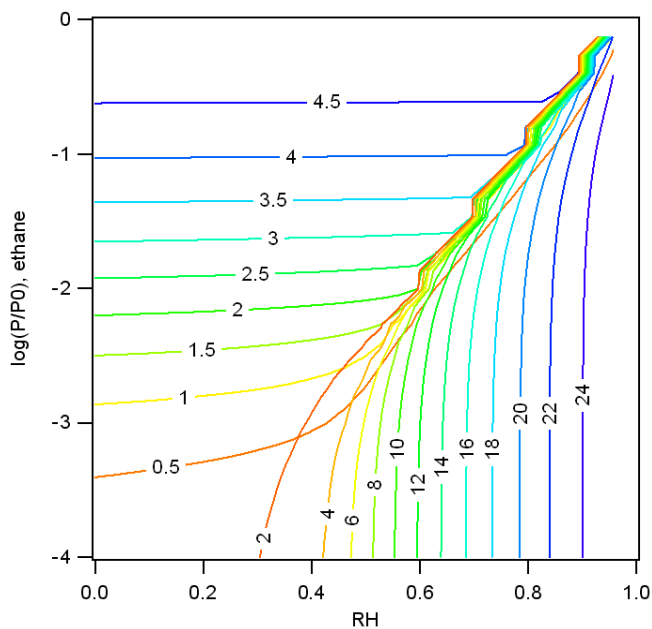


Figure 14. VGT prediction of the adsorption equilibrium of ethane-water mixtures on BPL carbon. Each line represents a fixed loading for ethane (top-left) and water (bottom-right).

Another interesting finding from the prediction is that the presence of water gives a sharp cut-out edge to the adsorption loading of non-polar organic compounds such as ethane. Figure 15 illustrates this idea. At a given partial pressure of ethane, as the relative humidity level increases, there is a turning point where the adsorption loading of ethane sharply decreases. As the partial pressure of ethane increases, this turning point of relative humidity shifts to higher value. This phenomenon has been widely recognized in previous experimental research, but cannot be properly modeled by traditional multi-component adsorption equilibrium model such as the modified D-R model developed by Wood.

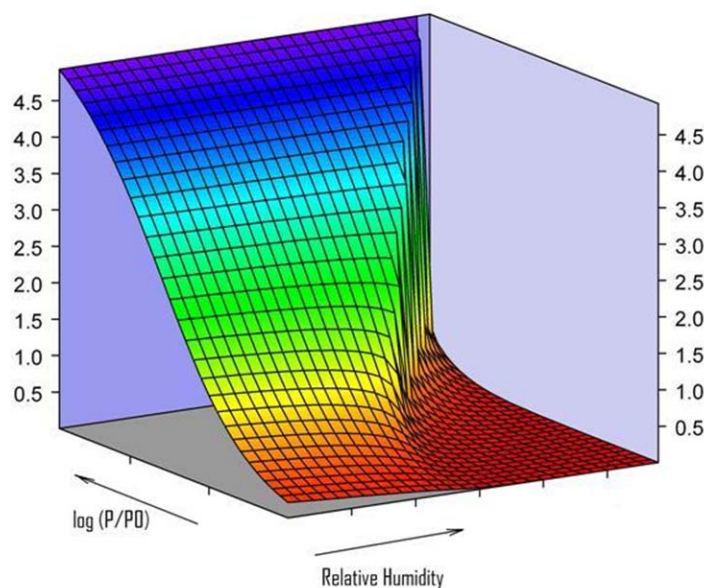


Figure 15. VGT prediction of the adsorption equilibrium of ethane-water mixtures on BPL carbon (3D view).

DISCUSSION

From the simulation results we have shown in the previous section, we find that the VGT method is capable of reasonably predicting the adsorption equilibrium of organic compounds, their mixtures, and their mixtures with water. This gives us a useful tool in the applications of the respiratory protection industry. The first application of the VGT method is the prediction of the service life of a respiratory cartridge for given use conditions such as the combination of contaminants, the variation of temperature, and the variation of humidity. This is particularly important in cases where service life time needs to be accurately calculated for a given use condition and it is very difficult to directly measure the adsorption equilibrium or the service life of a cartridge due to reasons like high toxicity.

Another potential application of the VGT method is to characterize an adsorbent by establishing the database of the VGT parameters. This will give one the convenience of estimating the adsorption equilibrium for numerous organic compounds. Also, it allows one to identify the adsorption characteristics of the adsorbent by analyzing the VGT parameters for different function groups, and to use this as an index to modify the adsorbent to target some particular types of chemicals.

In many cases adsorption is accompanied with catalytic reaction of the contaminants. Direct measurement of such reaction is impossible as they are conjugated with adsorption processes. For instance, it is hard to tell what portion of the contaminant is being adsorbed, and what portion of the contaminant is being hydrolyzed. While the VGT can predict reasonably well the adsorption portion, it is now possible to compare the predicted adsorption loading with the measured value of the loading, and estimate the portion that has been reacted. Combining this result with any detected reaction products, one can have a better understanding of the air purification mechanism. Such understanding will be useful in many cases such as new adsorbent development.

It should be noted that the VGT has been developed based on the assumption that the adsorption effect can be treated like the dilution of adsorbate with virtual groups. This assumption is good to some extent, but may not be appropriate for some situations. For example, if a significant portion of the pores of the adsorbent are smaller than the contaminant molecule sizes, physical limitations may exclude the contaminant molecules from entering the pore and thus cannot be treated as "mixed." The VGT will not be applicable to the adsorption process that is associated with reactions. Furthermore, if the adsorbent surface is strongly heterogeneous, it may not be appropriate to use a single virtual groups to represent the surface.

The virtual group density we collected from the probe chemical gets extremely high at the lower end. This means that certain high-energy adsorption sites exist but that they are not properly represented by the single virtual group. Consequently, the strong energy site is represented by the extraordinarily high density of the virtual group. Nevertheless, this deviation has limited effect on the prediction accuracy because the high energy surface sites are represented to some extent by the higher virtual group density. It is well known that the popular D-R equation used in the air purification industry is not thermodynamically consistent. It does not converge to a Henry's law limit when the contaminant concentration is extremely low. In such cases using the D-R equation may give a large error. The VGT, however, does not have this problem as it is developed based on the fugacity equation Eq. 1. This means that as the contaminant concentration approaches zero, the Henry's law limit is naturally achieved, which means good prediction may still be achieved in this ultra-low concentration limit.

Note that for the purpose of theoretical research, we simulate the concentrations and temperatures over a wide range. In the respiratory protection industry, the applicable concentration and temperature ranges may be narrower than those used in this research. Consequently, one can expect better prediction results given the less demanding ranges of concentrations and temperature.

Since the scope of this study is limited to fundamental theoretical research, we did not collect data for the VGT for a very wide extent of chemicals and conditions. Future research work is suggested to mature the VGT method and to identify the scope of its applications.

SUMMARY

We have presented a new group contribution method, namely the VGT method, for the prediction of adsorption equilibrium. Satisfactory results are achieved using the test chemicals in this research. The VGT provides a new way to predict adsorption equilibrium and hence the service life of respiratory cartridges. Also it can be used as an adsorbent characterization tool. The VGT may also be useful in some special research work such as the research of catalytic reactions associated with adsorption process. It is suggested that future research work be conducted to mature this technology and to identify its application scope.

Acknowledgement

The authors are grateful to the U.S. Army Edgewood Chemical Biological Center for financial support.

List of Symbols

A_{mn}	group interaction energy parameter of group m to group n
A_{vr}	group interaction energy parameter of the virtual group to a real group
n	adsorption loading, mol/kg
n_v	virtual group molar density, mol/kg
P	partial pressure of a chemical vapor, kPa
P_0	saturated vapor pressure of a chemical, kPa
R	UNIFAC group volume parameter
S	UNIFAC group surface parameter
T	temperature, K
X	mole fraction in a VLE equation
Γ	activity coefficient in a VLE equation

REFERENCES

- Appel WS, LeVan MD, and Finn JE, (1998). Nonideal adsorption equilibria described by pure component isotherms and Virial mixture coefficients. *Industrial and Engineering Chemistry, Research*, 37, 4774-4782.
- Ding Y, (2002). Periodic adsorber optimization and adsorption equilibrium measurement and prediction. Ph.D. Dissertation, Vanderbilt University.
- Eissmann RN, LeVan MD, (1993). Coadsorption of Organic Compounds and Water Vapor on BPL Activated Carbon. 2. 1,1,2-trichloro-1,2,2-trifluoroethane and dichloromethane. *Industrial & Engineering Chemistry Research* 36:2380--2389.
- Fredenslund A, Jones RL, Prausnitz JM, (1975). Group-contribution estimation of activity coefficients in nonideal liquid mixtures. *AIChE Journal*; 21:1086--1099.
- Fredenslund A, Gmehling J, Rasmussen P, (1977). *Vapor-liquid equilibria using UNIFAC*, Elsevier.
- Fu Y, Orbey H, Sandler SI, (1996). Prediction of vapor-liquid equilibria of associating mixtures with UNIFAC that include association. *Industrial & Engineering Chemistry Research*; 35, 4656-4666
- Gmehling J, Wittig R, Lohmann J, Joh R, (2002). A modified UNIFAC (Dortmund) model. 4. Revision and extension. *Industrial & Engineering Chemistry Research*, 41: 1678-1688.
- Hacskaylo JJ, (1987). Thermodynamic Studies of Vapor-Solid Adsorption Equilibria. Ph.D. Dissertation, University of Virginia.
- Horvath G and Kawazoe K, 1983. Method for the calculation of effective pore size distribution in molecular sieve carbon. *Journal of Chemical Engineering Japan* 1983, 16: 470-475.
- Lohmann JL, Joh R, Gmehling J, (2001). From UNIFAC to modified UNIFAC (Dortmund). *Industrial & Engineering Research*; 40, 957-964.
- Myers AL and Prausnitz JM, (1965). Thermodynamics of mixed-gas adsorption, *AIChE Journal*, 11, 121-127.
- Poling BE, Prausnitz JM, O'Connell JP, (2001). *The Properties of Gases and Liquids*, 5th ed. McGraw-Hill, Chapter 8.
- Rudisill EN, Hacskaylo JJ, LeVan MD, (1992). Coadsorption of organic compounds and water vapor on BPL activated carbon. *Industrial & Engineering Chemistry Research* 31:1122--1130.
- Rudisill EN, LeVan MD, (1992). Standard states for the adsorbed-solution theory. *Chemical Engineering Science*, 47:1239--1245.

-
- Russell BP, LeVan MD, (1996). Group contribution theory for adsorption of gas mixtures on solid surfaces. *Chemical Engineering Science* 51:4025--4038.
- Russell BP, LeVan MD, (1997). Coadsorption of organic compounds and water vapor on BPL activated carbon. 3. Ethane, propane, and mixing rules. *Industrial & Engineering Chemistry Research* 36:2380--2389.
- Spencer CF, Adler SB, (1978). A critical review of equations for predicting saturated liquid density. *Journal of Chemical Engineering Data* 23:82--89.
- Taqvi SM, Appel WS, and LeVan, MD, (1997). Virial description of two-component adsorption on homogeneous and heterogeneous surfaces. *Industrial & Engineering Chemistry, Research*, 36, 2197-2206.
- Taqvi SM, Appel WS, LeVan MD, (1999). Coadsorption of organic compounds and water vapor on BPL activated carbon. 4. Methanol, ethanol, propanol, butanol, and modeling. *Industrial & Engineering Chemistry Research* 38:240--250.
- Wood, GO, (1994). Estimating Service Lives of Organic Vapor Cartridges, *American Industrial Hygiene Association Journal* Jan: 11-15.
- Wood, GO, (1987a). A model for adsorption capacities of charcoal beds. I. Relative humidity effects. *American Industrial Hygiene Association Journal* 48: 622-625.
- Wood, GO, (1987b). A model for adsorption capacities of charcoal beds. II. Challenge concentration effects. *American Industrial Hygiene Association Journal* 48: 622-625.
- Wood, GO, (1992). Activated carbon adsorption capacities for vapors. *Carbon* 30: 593-599.
- Wood, GO, (2001). Affinity coefficients of the Polanyi-Dubinin adsorption isotherm equations - A review with compilations and correlations. *Carbon* 39: 343-356.
- Wood, GO, (2004). Estimating service lives of organic vapor cartridges II: a single vapor at all humidities. *Journal of Occupational and Environmental Hygiene* 1: 472-492.
- Wood, GO, (2005). Estimating service lives of air-purifying respirator cartridges for reactive gas removal. *Journal of Occupational and Environmental Hygiene* 2: 414-423.
- Wood, GO, (2007). Estimating service lives of organic vapor cartridges III: multiple vapors at all humidities. *Journal of Occupational and Environmental Hygiene* 4: 363-374.