THE INFLUENCE OF HUMIDITY ON THE ADSORPTION CAPACITY FOR ORGANIC VAPOURS OF AN ACTIVATED CARBON : A MATHEMATICAL MODEL

Peter Lodewyckx[1] and Jan Beirlant[2]

[1]Belgian Army - LogSpCxCENTRE-DTT/NBC-Division, Martelarenstraat 181, B-1800 Vilvoorde (Peutie)
[2]K.U. Leuven - Mathematics Dept, Celestijnenlaan 200B, B-3001 Heverlee

INTRODUCTION

One of the major problems faced by canister users is not being able to estimate the real life time of their carbon filters. Several authors have studied this problem and this resulted in a number of semi-empirical equations. One of the most widely used, in the case of pure physisorption, is the Wheeler-Jonas equation :

$$t_b = \frac{W_e \cdot W}{Q \cdot C_o} - \frac{\rho_b \cdot W_e}{k_v \cdot C_o} \cdot \ln\left(\frac{C_o - C_x}{C_x}\right) \qquad \text{(Eq.1)}$$

With :

- t_b = breakthrough time at C_x [min]
- W = weight of the carbon bed [g]
- W_e = adsorption capacity of the adsorbent for the chosen contaminant [$g_{contaminant}/g_{charcoal}$]
- Q = volumetric flow rate [cm^3/min]
- C_o = constant filter inlet concentration of the contaminant [g/cm^3]
- C_x = fixed concentration of the contaminant that defines breakthrough at the filter outlet [g/cm^3]
- ρ_b = apparent bulk density of the carbon [g/cm^3]
- k_v = overall adsorption rate coefficient [min^{-1}]

However, this simple but quite accurate [1,2,3], equation presents one major disadvantage : it can not be used to predict the life time of a filter in real circumstances as it is only valid for a non-humid carbon solicited by a dry contaminated airstream.

The only two parameters that are influenced by the (pre-)adsorbed water are W_e and k_v. So we tried to adapt the Wheeler-Jonas equation by using a W'_e and k'_v which correspond to the adsorption capacity and adsorption rate coefficient under well-defined humidity conditions. If it would be possible to express both W'_e and k'_v as a function of their values under dry conditions (W_e and k_v), the aging of the carbon (i.e. the amount of pre-adsorbed water) and the relative humidity of the airstream, one could use the Wheeler-Jonas equation for every given vapour, under any given circumstances.

EXPERIMENTAL

The activated carbon used was a BPL HA 12x30 from Chemviron. The bulk density of this carbon is 0.466 g/cm^3 and the micropore volume W_o, determined by N_2-adsorption on a Micromeritics ASAP 2010M, is 0.51 cm^3/g.

The carbon was challenged with seven different vapours :
Carbontetrachloride [CCl_4]
1,1,1-Trichloroethane [CH_3CCl_3]
Chlorobenzene [C_6H_5Cl]
n-Heptane [$CH_3(CH_2)_5CH_3$]
Cyclohexane [C_6H_{12}]
n-Butyl alcohol [$CH_3(CH_2)_3OH$]
1,2-Dichloroethane [$ClCH_2CH_2Cl$]
These substances were chosen because they are all non-soluble in water, and they present a wide range of values for the saturation pressure P_s [from 7 till 133 mbar] and molar polarisation P_e [from 11.0 till 34.6 cm^3/mol], both known to influence W_e and k_v.

Breakthrough tests were carried out on beds of 80 g of activated carbon (20 mm bed depth). The inlet concentration C_o was set at 5 g/cm^3 at a steady volumetric flow rate of 30 liters/min. The humidity of the airstream and the pre-wetting level of the carbon were varied between 0 and 90 % (at room temperature) to simulate different environmental conditions. All tests were performed in duplicate with an experimental error on the breakthrough time of maximum 15 %.
Two points of the breakthrough curve were determined by IR-spectroscopy : $C_x = 0.005$ g/m^3 and $C_x = 0.05$ g/m^3. This corresponds to the very first part of the breakthrough curve were a linear approximation is justified by experimental results.
This way one can calculate a W'_e and k'_v for every experiment [4].

Then we tried to find a mathematical model that expresses W'_e and k'_v as a function of the contaminant (through the parameters P_s and P_e) and the environmental conditions (pre-wetting H_{pw} and airstream humidity H_{air}).

RESULTS

All 136 experimentally-determined values of W'_e and k'_v were included in the mathematical model. This resulted in the following formula for W'_e :

$$\frac{W'_e}{W_e} = 1 + \frac{\tanh[b*(a-H_{air})]}{c} - d \qquad \text{(Eq. 2)}$$

With :

$$a = 1 - 0.07 * P_s^{0.3} - 0.3 * H_{pw}$$

$$b = 0.5 * P_s^{0.5} + \frac{2 * P_s}{P_e} * (H_{pw})^3$$

$$c = 27.7 - 15.2 * \left(\frac{P_s}{P_e}\right)^{0.22} - 0.02 * P_e^{1.6} * H_{pw}$$

$$d = 0.085 * \left(\frac{P_s}{P_e}\right)^{0.55} + 0.025 * P_s^{0.4} * P_e^{0.3} * (H_{pw})^{1.85}$$

In general the values of W'_e calculated with this formula are in good agreement with the experimentally determined values (See Fig 1 and 2 as examples involving CCl_4 and C_6H_5Cl : dotted and continuous lines represent calculated and experimental values respectively). At this stage we are still searching a similar expression for k'_v.

CONCLUSIONS

We were able to express W'_e as a function of environmental conditions. If a similar model can be obtained for k'_v one could use the Wheeler-Jonas equation to predict the breakthrough time of any given vapour, on any type of activated carbon, under any type of environmental circumstances.

REFERENCES

[1] G. Wood, *Am. Ind. Hyg. Assoc. J.* **55(1)**, 11 (1994)

[2] G. Wood, *Carbon* **30**, 593 (1992)

[3] G. Wood and J.F. Stampfer, *Carbon* **31**, 195 (1993)

[4] Odd Busmundrud, *Carbon* **31**, 279 (1993)

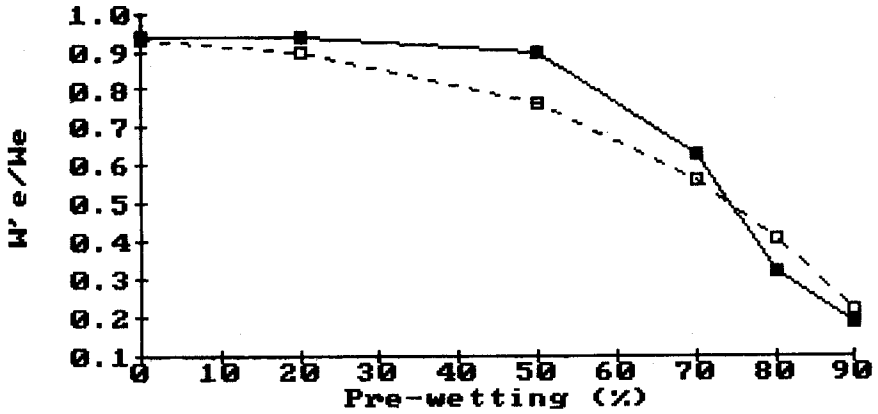

Fig 1 : CCl_4 in air with 50% Relative Humidity

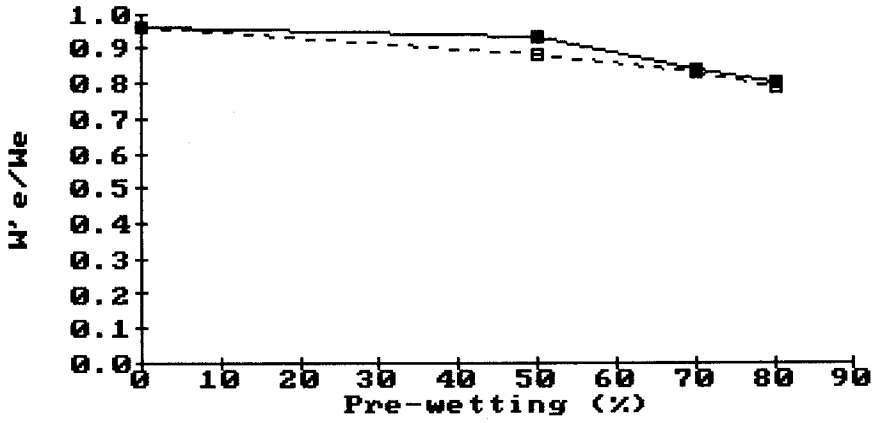

Fig 2 : C_6H_5Cl in air with 80% Relative Humidity