

Modelling the adsorption of styrene and acetone on activated carbon and perlite beds

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ABSTRACT

Experimental data from the Institute of Chemical Technology, Prague were analysed to derive some simple models of the rate of adsorption of either styrene or acetone from dilute air mixtures on sterile beds of activated carbon or perlite. It was found that the rate of progress towards the saturation of these beds could be reasonably accurately represented by a first order Lagergren model, where the rate constant had a value in the range 0.0039 to 0.29 min⁻¹.

1 INTRODUCTION

Biofiltration is a commonly used process to remove volatile organic compounds (VOC) from air streams (Gerrard *et al.*, 2005). It is particularly appropriate for applications with low inlet concentrations and high gas flows. The VOC is absorbed into a moist layer containing the micro-organisms and is biodegraded by them. In unsteady state conditions, adsorption onto the inert solid bed is also significant. In order to better understand this, the poster will describe the simple modelling of a number of experiments which measured the rate of adsorption of styrene and acetone (as both dry and moist gases) onto (biologically inactive) packed beds of activated carbon and of perlite.

2 EXPERIMENTAL

The beds were fed with a steady, incoming flow-rate of gases at a constant inlet concentration of solute. The inlet and outlet concentrations were measured. As time progressed, the bed became progressively saturated with the VOC, thus, the exit concentration steadily rose in a sigmoidal fashion. In total, fourteen experiments were carried out, (by varying the solute and the bed material, the inlet concentration level and the condition of the mixture at the inlet, (*i.e.* wet or dry).

3 THEORY

Where there was enough consistent data, the Freundlich isotherm:

$$q_e = mC_{in}^N \quad (1)$$

was used to represent the equilibrium data, where q_e = the (equilibrium) loading of solute on the bed divided by the bed mass, C_{in} = gas inlet concentration, and m and N are constants).

For the kinetic investigation, two models were used, the Lagergren and the Vermuelen.

Lagergren proposed to relate the total amount of solute adsorbed by the packing with time. He suggested the rate of change of adsorbed solids in the bed was proportional to the unsaturated state of the bed, raised to a power, thus:

$$\frac{dq}{dt} = k(q_e - q)^n \quad (2)$$

Here, q_e is the maximum (equilibrium) amount adsorbed per mass of bed, t is the time. k is the adsorption rate constant (k_1 for pseudo first order and k_2 for the pseudo second order approach) and n is the model's order. This equation is easily solved for $n = 1$ and $n = 2$. For the pseudo first order model ($n = 1$) the equation gives:

$$\ln(q_e - q) = \ln q_e - k_1 t \quad (3)$$

For the pseudo second order model ($n = 2$) the equation gives:

$$\frac{t}{q} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t \quad (4)$$

Clearly, both equations are easily linearised.

Vermuelen (1953) proposed an equation to describe the fraction of adsorbed solute compared to equilibrium as a function of time, ($F(t)=q/q_e$). He formulates his equation thus:

$$F(t) = \left[1 - \exp\left(\frac{-Dt\pi^2}{r_0^2}\right) \right]^{0.5} \tag{5}$$

where D= effective particle diffusivity and r_0 is the particle size. We can define.

$$A = \frac{D\pi^2}{r_0^2}$$

Then substitution and rearrangement lead to a straight line formula:

$$\ln\left(\frac{1}{1 - F(t)^2}\right) = At \tag{6}$$

This can be plotted so that the slope gives A directly.

4 RESULTS

For the equilibrium data, the styrene-perlite experiments were the most consistent and gave the following logged graph, see Figure 1, for the five experimental runs. For the dry system, the Freundlich equation has an index of around 1.4 and for the wet conditions, it was closer to unity.

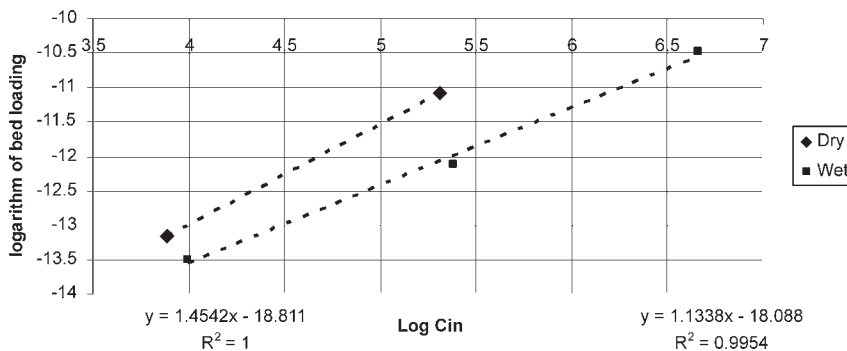


Figure 1. Freundlich diagram for styrene on perlite.

Moving to the modelling of the kinetic data, Figures 2 and 3 show log- linear plots showing the above styrene on perlite data fitted to a pseudo first order Lagergren model:

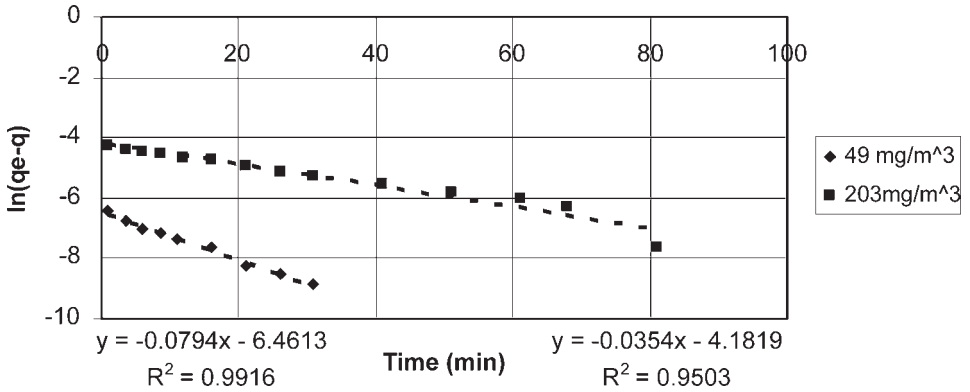


Figure 2. First order Lagergren model for styrene on dry perlite.

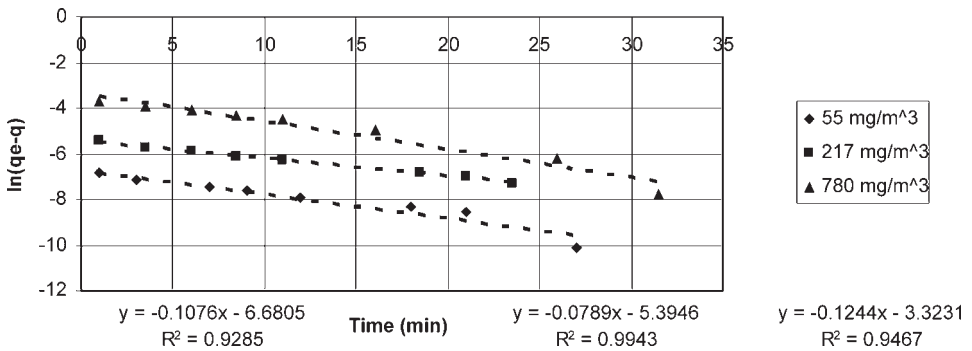


Figure 3. First order Lagergren model on wet perlite.

All the coefficients of determination are well above 90%, indicating a reasonable fit.

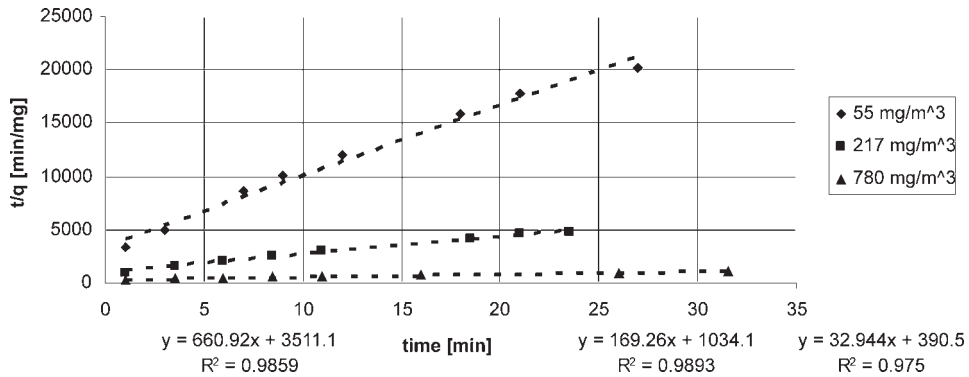


Figure 4. Second order Lagergren model for styrene on wet perlite.

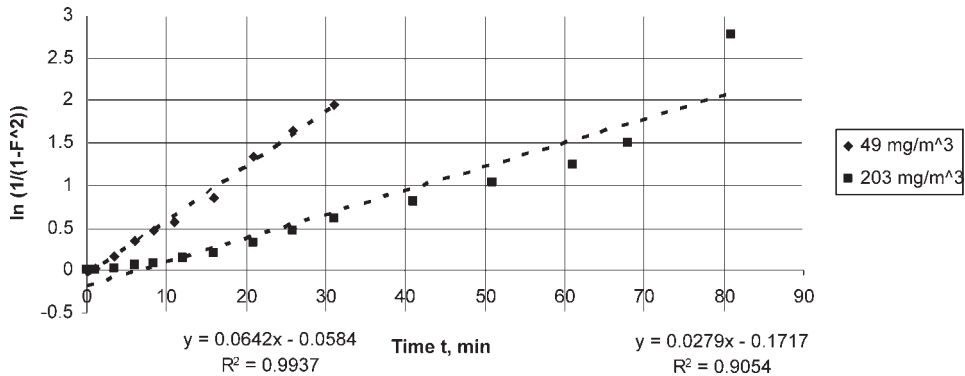


Figure 5. Vermeulen model for styrene on dry perlite.

Figures 4 and 5 show another pair of graphs where some of the styrene on perlite data is fitted to the other two models. Again, the goodness of fit values are pleasing.

The Table 1 below summarises all 14 experimental runs and lists the kinetic parameters (k_p , k_2 and A) and the coefficient of determination, R^2 , for the three models tested. For example, the third, fourth and fifth rows of numerical data, show the effect of changing inlet concentration for the wet styrene on perlite system.

As noted above, all three approaches give reasonable fits to the data, with the average R^2 value being 93% for the first order Lagergren model, 88% for the Vermeulen and 86% for the second order Lagergren model. In addition, the range of values of the constants is somewhat smaller for the first order model, which is a further reason to (slightly) prefer it to the alternatives.

In more detail: we note for the styrene on perlite results that the inlet concentration does not have a large effect on the value of k_p , especially for the wet system. The results for wet acetone on perlite also give almost constant values for this parameter.

Table 1.
Summary of the constants found in the three models.

Inlet Concentration	k_1	R^2	k_2	R^2	A	R^2
	Lagergren	First order	Lagergren	2 nd order	Vermeulen	model
Dry styrene on perlite						
49	0.079	0.992	83.5	0.997	0.064	0.994
203	0.035	0.950	3.24	0.986	0.028	0.905
Wet styrene on perlite						
55	0.11	0.929	151.	0.986	0.089	0.900
217	0.079	0.994	31.9	0.989	0.06	0.989
780	0.12	0.947	3.22	0.975	0.10	0.900
Dry styrene on carbon						
2498	0.049	0.964	0.016	0.967	0.043	0.933
928	0.0069	0.741	0.000041	0.572	0.0052	0.653
Wet styrene on carbon						
693	0.0039	0.985	0.00019	0.916	0.0041	0.845
Dry acetone on perlite						
645	0.085	0.865	0.261	0.452	0.072	0.816
1677	0.29	0.979	6.56	0.792	0.23	0.960
Wet acetone on perlite						
920	0.044	0.987	0.0266	0.966	0.039	0.964
2517	0.047	0.963	0.015	0.968	0.041	0.932
Dry acetone on carbon						
929	0.0069	0.741	0.00004	0.5724	0.0052	0.653
Wet acetone on carbon						
681	0.0041	0.983	0.00021	0.936	0.0042	0.861

5 CONCLUSIONS

It was found that the pseudo first order Lagergren model gave a good fit to most of the data. Typically, the values for k_1 ranged from around 0.0039 to 0.29 min^{-1} and the coefficients of determination were usually over 90%.

6 NOMENCLATURE

A	constant
C	concentration
D	diffusivity
F	fractional saturation of bed
k	rate constant
m	equilibrium constant
n	order of model
N	power in Freundlich equation
q	solute adsorbed on bed
r_o	radius of pore
R^2	coefficient of determination
t	time

subscripts

e	equilibrium
in	inlet condition

REFERENCES

- Gerrard, A.M., Misiaczek, O., Hajkova, D., Halecky, M. and Paca, J. (2005) Steady state models for the biofiltration of styrene/air mixtures. *Chemical and Biochemical Engineering Quarterly*. 19 (2): 185-190.
- Vermuelen, T. (1953) Theory for Irreversible and Constant- Pattern Solid Diffusion. *Industrial and Engineering Chemistry*. 45: 1664-1665.