

MODELLING OF SINGLE GAS SORPTION PROCESSES IN SHALLOW FIXED BED ADSORBERS

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Introduction

The objective of this work was to simulate the adsorption process of gases in a filter bed of activated carbon, mainly focussed on the application to gasmask canisters. The model was validated by comparison of the simulation results with experimental results on the adsorption of toluene at ambient temperature in a shallow packed bed of activated carbon.

Mathematical model

The transport mechanism in the gas phase was described by a dispersed plug flow model accounting for mixing in the axial direction. The resistance for mass transfer between the bulk of the gas phase and the outer surface of the particle was located in a fictitious film around the particle. Intraparticle gas transport was described by a diffusive contribution assuming Ficks law and an effective molecular diffusion coefficient as transport parameter. Equilibrium between the gas phase and solid phase concentrations was assumed at each position throughout the particle. Both phases were assumed to be isothermal.

The continuity equation for the adsorptive over the gas phase is given by:

$$\varepsilon_b \frac{\partial C_b}{\partial t} = D_{ea} \frac{\partial^2 C_b}{\partial z^2} - u_s \frac{\partial C_b}{\partial z} - (1 - \varepsilon_b) k_f a (C_b - C_i)$$

where C_b is the bulk gas phase concentration, u_s is the superficial gas velocity, D_{ea} is the effective axial diffusion coefficient, z is the axial coordinate, ε_b is the bed porosity, a is the external surface area per unit particle volume and k_f is the mass transfer coefficient.

Assuming spherical particles, and assuming local equilibrium in the particles, the continuity equation for the adsorptive over the solid phase is given by:

$$\left(\frac{\partial q}{\partial C_p} + \varepsilon_p \right) \frac{\partial C_p}{\partial t} = \frac{D_{eff}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_p}{\partial r} \right)$$

where C_p is the intraparticle gas phase concentration, q is the adsorptive loading, ε_p is the particle porosity, D_{eff} is the effective molecular diffusion coefficient and r is the radial coordinate inside the particle. The following boundary conditions were used:

$$D_{eff} \frac{\partial C_p}{\partial r} \Big|_{r=r_p} = k_f (C_b - C_i) \quad \text{and} \quad \frac{\partial C_p}{\partial r} \Big|_{r=0} = 0$$

The Dubinin-Radushkevich adsorption isotherm was applied to describe the equilibrium sorption data of toluene on activated carbon:

$$\frac{q}{q_{max}} = \exp \left(- \left(\frac{RT}{\beta E_0} \right)^2 \ln^2 \left(\frac{c}{c_s(T)} \right) \right)$$

The values of the parameters E_0 en q_{max} were estimated by regression of this equation to the experimental isotherm data of toluene for a calculated value of β (Duisterwinkel¹).

The set of partial differential equations and corresponding initial and boundary conditions was solved numerically by discretisation of the equations (method of lines) followed by integration of the set of ordinary differential equations using a standard numerical integration routine for stiff problems with a sparse Jacobian.

Model parameters

The values of the parameters used in the simulations are shown in Table 1. The gas mixture consists of nitrogen and toluene, the latter present in very low concentrations. Therefore the physical

parameters of the gas mixture are based on the values of pure nitrogen. The effective axial diffusion coefficient (Gunn²) and mass transfer coefficient (Dwivedi and Upadhyay³) were calculated from correlations for classical fixed beds. Variables in the simulations were the bed length, 0.01 to 0.035 m, the superficial gas velocity, 0.127 to 0.191 m³ m⁻² r s⁻¹ and the toluene inlet concentration, 1.11 10⁻³ to 4.83 10⁻³ kg m⁻³ f. The adsorbent used in the experiments was Norit R1 activated carbon (Norit N.V., The Netherlands), which has a bimodal pore size distribution with both macro- and micropores. During the experiments the activated carbon was placed in a quartz tube with a precision diameter of 0.05 m.

Table 1. Parameter values used in the simulation of the sorption process of toluene in a shallow packed bed of activated carbon

	Value	Unit		Value	Unit
q_{max}	324	kg m ⁻³ pt	D_{eff}	8.8 10 ⁻⁶	m ³ m ⁻¹ pore s ⁻¹
E_o	16065	J mol ⁻¹	ϵ_b	0.372	m ³ m ⁻³ r
β	1.194	--	ϵ_p	0.55	m ³ m ⁻³ pt
d_{pt}	1.2 10 ⁻³	m _{pt}	Pe_{ax}	2	-
C_{sat}	0.125	kg m ⁻³ f	ρ_{gas}	1.18	kg m ⁻³
T	298	K	μ_{gas}	1.8 10 ⁻⁵	kg m ⁻¹ s ⁻¹

Results and Discussion

Typical results for calculated and experimentally determined outlet concentrations of toluene as a function of time are shown in Figure 1 and 2 for different bed lengths. The symbols refer to experimentally determined outlet concentrations while the solid lines refer to simulated values.

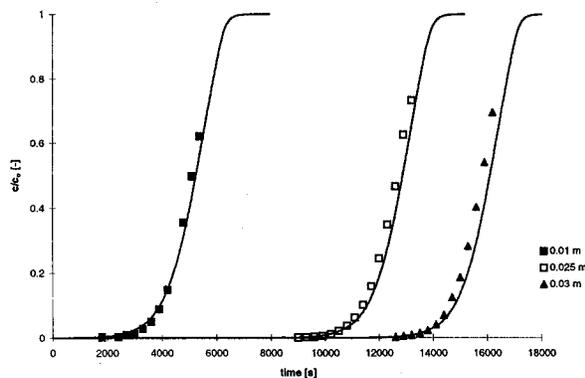


Figure 1. Normalised outlet concentrations of toluene as a function of time when continuously feeding a mixture of toluene and nitrogen to a packed bed of activated carbon with $C_o = 2.25 \cdot 10^{-3} \text{ kg m}^{-3} \text{ f}$ and $u_s = 0.127 \text{ m}^3 \text{ m}^{-2} \text{ r s}^{-1}$.

In Figure 2 the y-axis is shown on a semilogarithmic scale to allow a better comparison at low normalised toluene concentrations.

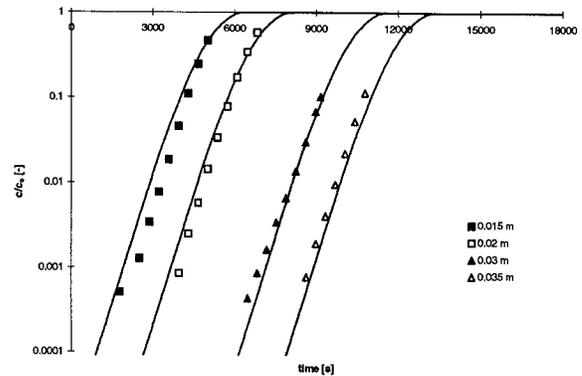


Figure 2. Normalised outlet concentrations of toluene as a function of time when continuously feeding a mixture of toluene and nitrogen to a packed bed of activated carbon with $C_o = 2.35 \cdot 10^{-3} \text{ kg m}^{-3} \text{ f}$ and $u_s = 0.191 \text{ m}^3 \text{ m}^{-2} \text{ r s}^{-1}$.

The agreement between purely calculated and experimentally determined toluene outlet concentrations is good, though it is slightly less at low concentrations. The model is able to account well for changes in the mass transport rates due to changes in the superficial gas velocity and toluene inlet concentration.

Simulations are currently being carried out to investigate the influence of different filter geometries and variations in the superficial gas velocity, *i.e.* respiration patterns, on the breakthrough behavior of organic components.

Conclusions

A mathematical model was developed to simulate the sorption process of toluene in shallow packed beds of activated carbon. The values of the transport parameters were estimated from correlations for classical fixed beds. A good agreement was obtained between calculated and measured toluene outlet concentrations at varying bed length, superficial gas velocity and toluene inlet concentration.

References

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3. Dwivedi, P.N. and Upadhyay, S.N., *Ind. Eng. Chem., Process Des. Dev.*, 1977, 16(2), 157.