

# ANOXIC DIFFUSION OF PHENOLIC COMPOUNDS IN GRANULATED ACTIVATED CARBON: BATCH STUDIES

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## Introduction

The mechanism of adsorption of phenolic compounds on granular activated carbons(GAC) is complex. The problem is that most experimental measurements involve large integral steps in either well stirred mixed baths or in columns(1). Modeling these experiments involves a complex combination of thermodynamics (isotherm), and rate processes (pore and surface diffusion which may be concentration dependent(2)). In this paper, the adsorption is modeled using the chemical potential as driving force for the surface transport into the GAC combined with the Langmuir-Freundlich isotherm. The flux is taken as a dual mechanism of pore and surface diffusion .

## Experimental

A finite bath of 4 liter volume is loaded with GAC particles of constant size 0.156 cm. The particles are suspended in a wire mesh container in the bath to maximize the fluid velocity over the particles to reduce the film mass transfer resistance. The liquid phase consists of water plus the dissolved phenolic organic, and was neutralized with a buffer to a pH of 7.0 The bath contained an impeller and four baffles. The rate of rotation of the impeller was made sufficiently high so that no film mass transfer resistance could be detected. Samples of the liquid phase were analyzed periodically for the organic(3).

## Theoretical

The following assumptions are made :

- (i) the bath is finite,
- (ii) the system is at constant temperature,
- (iii) the adsorbent particles are isotropic with uniform pores and no preferential pore direction,
- (iv) the solution is dilute so that the molecular diffusivity and the mass transfer coefficient are constant
- (v) the bath is stirred sufficiently such that the film transport is negligible in comparison to the other resistances.
- (vi) the organic diffuses by a combined surface and pore diffusion mechanism. The surface diffusion driving force is the chemical potential gradient and the relationship expressing the diffusion coefficient for the adsorbed species is given by Darken's relation

$$D_s = D_{s0} \frac{\partial \ln C}{\partial \ln q}$$

Assuming the combined pore and surface flux to be :

$$N = -(\varepsilon D_p \frac{\partial C_p}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r})$$

the particle mass balance gives, neglecting accumulation in the pores

$$\rho_p \frac{\partial q}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left\{ r^2 \left[ \varepsilon D_p \frac{\partial C_p}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r} \right] \right\}$$

$$\text{As } \frac{\partial C_p}{\partial r} = \frac{\partial C_p}{\partial q} \frac{\partial q}{\partial r}$$

our adsorption equation can be rearranged to give

$$\rho_p \frac{\partial q}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left\{ r^2 \left[ \varepsilon D_p \frac{\partial C_p}{\partial q} + \rho_p D_s \right] \frac{\partial q}{\partial r} \right\}$$

where  $\frac{\partial C_p}{\partial q}$  is obtained from the isotherm equation used.

**Initial conditions :**

$$\begin{aligned} C &= C_o; & r &= 0 \\ C_p &= C_p(\tau, 0) = 0; & 0 \leq r \leq r_s \\ q(r, 0) &= 0; & 0 \leq r \leq r_s \end{aligned}$$

**Boundary conditions**

$$\left. \frac{\partial q(0, t)}{\partial r} \right|_{r=0} = 0 \quad \left. \frac{\partial C_p}{\partial r} \right|_{r=0} = 0$$

$$V(C_o - C) = \int_0^r (-4\pi r^2 n \rho_p D_{eff} \cdot \left. \frac{\partial q}{\partial r} \right|_{r=r_s}) dt$$

where  $D_{eff} = \varepsilon \frac{D_p}{\rho_p} \frac{\partial C_p}{\partial q} + D_s$

and  $4\pi r_s^2 n = \frac{3V_s}{r_s}$

The isotherms for the phenolic compounds were expressed by

$$\frac{q_A}{q_{Asat}} = \frac{k_A C_A^{1/na}}{1 + k_A C_A^{1/na}}$$

These equations were normalized and solved using Crank-Nicholson finite difference scheme employing 50 grid points.

## Results and Discussion

Five different models were tested using these equations:

- (1) Pore diffusion model only(PDM).
- (2) Homogeneous surface diffusion model (HSDM) with  $D_s$  constant
- (3) HSDM model with concentration dependent surface diffusivity.
- (4) Combined pore and surface diffusion model (CPSDM) with  $D_s$  constant.
- (5) CPDSM model with concentration dependent surface diffusivity.

The best fit of the data was found with model 5 for which the results are presented in Figures 1 and 2. However, the RMS fit was found to be highly temperature dependent indicating that the choice of isotherm model is critical.

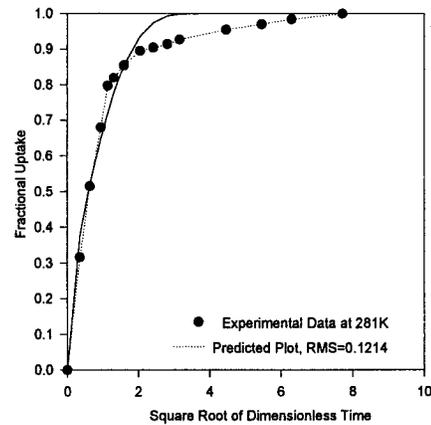


Figure 1. Adsorption of Phenol at 281K : Experimental and Predicted Uptake.

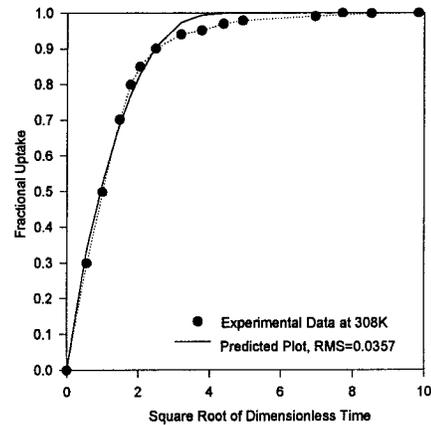


Figure 2. Adsorption of o-cresol at 308K : Experimental and Predicted Uptake.

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## References

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