

# ADSORPTION OF MULTIPLE CONTAMINANTS FROM A FLUID STREAM

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## Abstract

We develop a mathematical model to describe an adsorption process in which two species compete to occupy the available sites on the adsorbing particles. The governing equations consist of a standard advection-diffusion and a kinetic equation for each species, the latter consisting of two groups of terms: one related to individual adsorption processes and the second describing all the interaction between the two species. Once the relevant variables are scaled and the dimensionless parameters have been identified, the system is solved numerically and validated against experimental data.

## 1 Introduction

One practical method of removing a contaminant from a carrier fluid is column sorption, either through absorption or adsorption. Column sorption involves passing a fluid through a tube filled with a material capable of capturing certain components of the fluid. The mathematical model for describing the adsorption process of a

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single contaminant has been widely studied in recent years, see [1, 2, 3, 4]. However, a carrier fluid typically contains more than one contaminant which results in significantly more complicated kinetics [5, 6, 7]. Mathematically, the process is also much more complicated since multiple moving boundaries may exist while interaction, due to the competition for adsorbent sites, must be accounted for. The process is depicted in Figure 1, where a mixture of a carrier gas (green molecules) and two contaminants (blue and red molecules) are introduced at the column inlet and then start attaching to the adsorbent. While this occurs, the contaminants compete with each other and may displace each other from occupied sites.

To be able to develop a correct mathematical model that accounts for individual and competitive adsorption, we will first discuss the relevant chemical reactions and will then extend the recently validated model discussed in [4]. To reduce the complexity of this first study, we will focus on the case where 2 contaminants are present and where one is dominant (meaning that it displaces the other, but is not itself displaced).

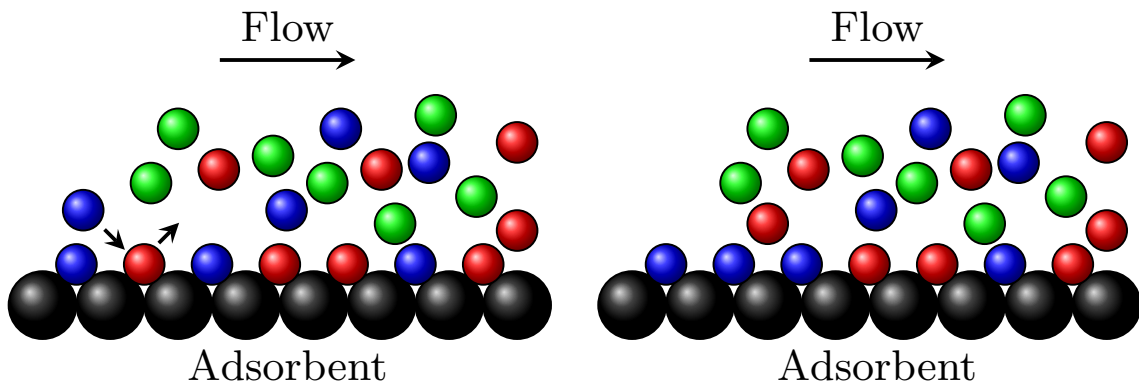


Figure 1: Schematic of the competitive adsorption process. Here, the blue contaminant is displacing a previously adsorbed red molecule.

## 2 Key variables

The concentration per unit length of each contaminant in the fluid will be denoted by  $c_i$ . This variable represents the average over a cross-section of the column, the averaging process is detailed in [4, 9].

The adsorbed material is typically described by the contaminant adsorbed per mass of adsorbent, represented by  $q$ . However, when competition occurs for the available sites it turns out more convenient to work in terms of the fractional coverage of the adsorbent surface by a monolayer of adsorbate, represented by  $\theta = q/q_m$ , where  $q_m$  is the maximum adsorbate loading. For multiple components we write  $\theta_i = q_i/q_{m,i}$ , where different  $q_{m,i}$  mean that the maximum mass that the adsorbent

can retain is different for each species (if the number of sites is fixed and the contaminant molecules have a different weight then the total adsorbed mass will change depending on which molecule occupies the sites).

### 3 Chemical reactions

We consider three reactions, in the first  $c_1$  attaches to the adsorbent material at a rate  $k_{ad,1}$ , it may also desorb at a rate  $k_{de,1}$ . A similar reaction occurs with  $c_2$ . These are standard adsorption reactions. Finally there is a displacement reaction where  $c_1$  replaces adsorbed  $c_2$  or  $c_2$  replaces adsorbed  $c_1$ , with a rate denoted by  $k_{re}$ . The resultant system is

- Reaction 1:  $c_1 + \mathbf{A} \xrightleftharpoons[k_{de,1}]{k_{ad,1}} c_1\mathbf{A}$ ;  $r_1 = k_{ad,1}c_1(1 - \theta_1 - \theta_2) - k_{de,1}\theta_1$
- Reaction 2:  $c_2 + \mathbf{A} \xrightleftharpoons[k_{de,2}]{k_{ad,2}} c_2\mathbf{A}$ ;  $r_2 = k_{ad,2}c_2(1 - \theta_1 - \theta_2) - k_{de,2}\theta_2$
- Reaction 3:  $c_1 + c_2\mathbf{A} \xrightleftharpoons[k_{re,2}]{k_{re,1}} c_1\mathbf{A} + c_2$ ;  $r_3 = k_{re,1}c_1\theta_2 - k_{re,2}c_2\theta_1$

Note, that it is convenient to define the rate of reaction 3 in both directions, depending on which is the free component where it starts from. Hence,  $k_{re,1}$  is the rate by which free  $c_1$  replaces the already adsorbed  $c_2\mathbf{A}$  and  $k_{re,2}$  is the rate at which  $c_1\mathbf{A}$  is displaced by free  $c_2$ . To focus only on the case where  $c_1$  is dominant such that it displaces nearly all  $c_2$ , we will assume  $k_{re,2} = 0$ .

### 4 Mathematical model

The mathematical description of the adsorption problem with two contaminants will be based on the model for one contaminant studied in [2, 3, 4].

For each individual contaminant  $i$ , the mass balance is defined by the advection-diffusion equation

$$\frac{\partial c_i}{\partial t} + u \frac{\partial c_i}{\partial x} = D \frac{\partial^2 c_i}{\partial x^2} - \alpha_i \frac{\partial \theta_i}{\partial t} \quad (i = 1, 2), \quad (4.1)$$

where  $\alpha_i$  denotes the rate at which  $c_i$  attaches to the surface, with a conversion factor reflecting the fact that  $c_i$  is a mass density, while  $\theta_i$  is a fraction of occupied sites. Equation (4.1) is coupled to the adsorption equations derived from the above reaction system,

$$\frac{\partial \theta_1}{\partial t} = r_1 + r_{1,2} = k_{ad,1}c_1(1 - \theta_1 - \theta_2) - k_{de,1}\theta_1 + k_{re,1}c_1\theta_2, \quad (4.2a)$$

$$\frac{\partial \theta_2}{\partial t} = r_2 + r_{2,1} = k_{ad,2}c_2(1 - \theta_1 - \theta_2) - k_{de,2}\theta_2 - k_{re,1}c_1\theta_2. \quad (4.2b)$$

The problem is closed by writing the boundary and initial conditions, which are

$$uc_{i,in} = uc_i - D \frac{\partial c_i}{\partial x}, \quad x = 0, \quad (4.3a)$$

$$\frac{\partial c_i}{\partial x} = 0, \quad x = L, \quad (4.3b)$$

$$c_i, \theta_i = 0, \quad t = 0. \quad (4.3c)$$

Once a mathematical problem is defined, the relevant quantities are typically scaled to obtain a non-dimensional model showing the relative importance of each term. We choose the following scaled variables,

$$c_i = c_{i,in} \bar{c}_i, \quad t = \tau \bar{t}, \quad x = \mathcal{L} \bar{x}, \quad (4.4)$$

where  $\tau$  and  $\mathcal{L}$  are two unknown scales which will be defined below. Note, the fraction of occupied sites  $\theta_i$  are already scaled. For each contaminant  $i$ , the advection-diffusion equation becomes

$$\text{Da} \frac{\partial \bar{c}_i}{\partial \bar{t}} + \frac{\partial \bar{c}_i}{\partial \bar{x}} = \text{Pe}^{-1} \frac{\partial^2 \bar{c}_i}{\partial \bar{x}^2} - \frac{\alpha \mathcal{L}}{uc_{i,in} \tau} \frac{\partial \theta_i}{\partial \bar{t}}, \quad (4.5)$$

where we have introduced the non-dimensional Damköhler and inverse Péclet numbers

$$\text{Da} = \frac{\mathcal{L}}{\tau u}, \quad \text{Pe}^{-1} = \frac{D}{\mathcal{L} u}. \quad (4.6)$$

The form of eq. (4.5) suggests that each contaminant has a characteristic length scale  $\mathcal{L}_i = uc_{i,in} \tau / \alpha_i$ .

On the other hand, the kinetic equations become

$$\frac{1}{\tau} \frac{\partial \theta_1}{\partial \bar{t}} = k_{ad,1} c_{1,in} \bar{c}_1 (1 - \theta_1 - \theta_2) - k_{de,1} \theta_1 + k_{re,1} c_{1,in} \bar{c}_1 \theta_2, \quad (4.7a)$$

$$\frac{1}{\tau} \frac{\partial \theta_2}{\partial \bar{t}} = k_{ad,2} c_{2,in} \bar{c}_2 (1 - \theta_1 - \theta_2) - k_{de,2} \theta_2 - k_{re,1} c_{1,in} \bar{c}_1 \theta_2. \quad (4.7b)$$

As the primary focus is adsorption and we have defined contaminant 1 as the dominant one, we will choose  $\tau = 1/(k_{ad,1} c_{1,in})$ . Similarly we choose  $\mathcal{L} = \mathcal{L}_1$  to yield the governing equations

$$\text{Da} \frac{\partial \bar{c}_1}{\partial \bar{t}} + \frac{\partial \bar{c}_1}{\partial \bar{x}} = \text{Pe}^{-1} \frac{\partial^2 \bar{c}_1}{\partial \bar{x}^2} - \frac{\partial \theta_1}{\partial \bar{t}}, \quad (4.8a)$$

$$\text{Da} \frac{\partial \bar{c}_2}{\partial \bar{t}} + \frac{\partial \bar{c}_2}{\partial \bar{x}} = \text{Pe}^{-1} \frac{\partial^2 \bar{c}_2}{\partial \bar{x}^2} - \delta \frac{\partial \theta_2}{\partial \bar{t}}, \quad (4.8b)$$

$$\frac{\partial \theta_1}{\partial \bar{t}} = \bar{c}_1 (1 - \theta_1 - \theta_2) - \kappa_1 \theta_1 + \beta \bar{c}_1 \theta_2, \quad (4.8c)$$

$$\gamma \frac{\partial \theta_2}{\partial \bar{t}} = \bar{c}_2 (1 - \theta_1 - \theta_2) - \kappa_2 \theta_2 - \gamma \beta \bar{c}_1 \theta_2, \quad (4.8d)$$

where

$$\delta = \frac{\mathcal{L}_1}{\mathcal{L}_2} = \frac{c_{1,in}}{c_{2,in}}, \quad \gamma = \frac{k_{ad,1}c_{1,in}}{k_{ad,2}c_{2,in}}, \quad \kappa_i = \frac{k_{de,i}}{k_{ad,i}c_{i,in}}, \quad \beta = \frac{k_{re,1}}{k_{ad,1}}. \quad (4.9)$$

Finally, the non-dimensional boundary and initial conditions are

$$1 = \bar{c}_i - \text{Pe}^{-1} \frac{\partial \bar{c}_i}{\partial \bar{x}}, \quad \bar{x} = 0, \quad (4.10a)$$

$$\frac{\partial \bar{c}_i}{\partial \bar{x}} = 0, \quad \bar{x} = \bar{L}, \quad (4.10b)$$

$$\bar{c}_i, \theta_i = 0, \quad \bar{t} = 0, \quad (4.10c)$$

where  $\bar{L} = L/\mathcal{L}_1$ .

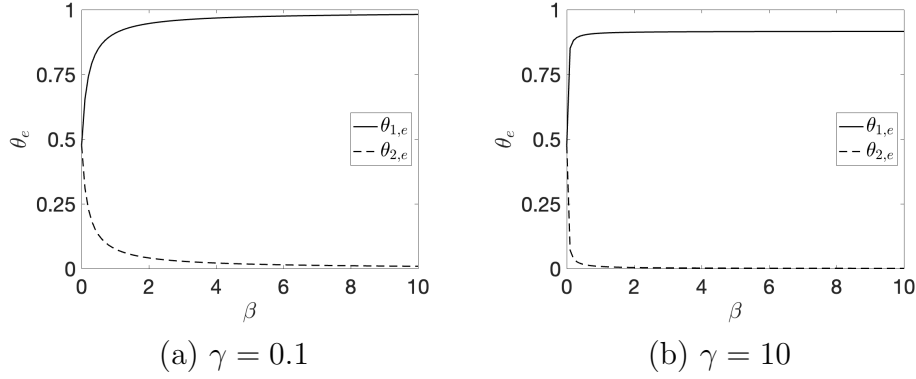


Figure 2: Dependence of the equilibrium values  $\theta_{i,e}$  on  $\beta$ , for different values  $\theta_{i,e}$ . can then be found by solving the linear system  $\lambda$ .

When equilibrium is reached and adsorption balances desorption the time derivatives in eqs. (4.8c) and (4.8d) become zero,  $\bar{c}_i \rightarrow 1$  and  $\theta_i \rightarrow \theta_{i,e}$ . The equilibrium values  $\theta_{i,e}$  can then be found by solving the linear system

$$\begin{pmatrix} 1 + \kappa_1 & 1 - \beta \\ 1 & 1 + \kappa_2 + \gamma\beta \end{pmatrix} \begin{pmatrix} \theta_{1,e} \\ \theta_{2,e} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (4.11)$$

An example of the variation of  $\theta_{i,e}$  against  $\beta$  is shown in Fig. 2. The parameter  $\beta = k_{re,1}/k_{ad,1}$  represents the ratio of the replacement rate to the adsorption rate of contaminant 1. Here we keep  $k_{ad,1}$  fixed (since this affects  $\kappa_1$ ) so that the  $\beta$  variation strictly reflects a change in the replacement rate. We choose  $\kappa_1 = \kappa_2 = 0.1$  and then when  $\beta = 0$  both adsorption sites take the value 0.1/0.21. As the value of  $\beta$  increases, so that contaminant 2 is replaced to a greater extent, the equilibrium value of  $\theta_1$  increases while that of  $\theta_2$  decreases. Increasing  $\gamma \propto k_{ad,1}$  affects the rate the asymptote is approached but also the value of the asymptote. As  $\beta \rightarrow \infty$ ,  $\theta_{1,e} \rightarrow (1 + \gamma)/(1 + \gamma(1 + \kappa_1)) \approx 0.991, 0.92$  for the two cases shown, while  $\theta_{2,e} \rightarrow \kappa_1/(\beta(1 + \gamma(1 + \kappa_1))) \approx 0$ .

## 5 Results

Typically, single contaminant column adsorption/desorption problems can be solved analytically using the travelling wave method [2, 3, 4, 8]. However, the problem defined by eqs. (4.8) and (4.10) is a system of 4 coupled equations and therefore in general difficult to solve analytically (the travelling wave approach was attempted but it did not seem to work in this case). Nonetheless, the possibility of obtaining analytical solutions will be explored in future work. Due to the difficulty of deriving an analytical solution and the time constraints of the study group, the system was solved numerically using the software *Matlab*.

In the following work the data used comes from the LEQUIA laboratory, see [5] and concerns the adsorption of two volatile methyl siloxanes: a linear molecule, hexamethyldisiloxane (L2) and a cyclic one, octamethylcyclotetrasiloxane (D4). These are common low concentration water contaminants.

Equation (4.11) defines the equilibria, which may be written in dimensional form as

$$\theta_{e,1} = \frac{K_1 c_{e,1} \left(1 + \frac{K_2}{K_{3,2}} c_{e,1} + \frac{K_2}{K_{3,1}} c_{e,2}\right)}{1 + K_2 c_{e,2} \left(1 + \frac{K_1}{K_{3,1}} c_{e,1}\right) + c_{e,1} \left[\frac{K_2}{K_{3,2}} + K_1 \left(1 + \frac{K_2}{K_{3,2}} c_{e,1}\right)\right]}, \quad (5.1)$$

$$\theta_{e,2} = \frac{K_2 c_{e,2}}{1 + K_2 c_{e,2} \left(1 + \frac{K_1}{K_{3,1}} c_{e,1}\right) + c_{e,1} \left[\frac{K_2}{K_{3,2}} + K_1 \left(1 + \frac{K_2}{K_{3,2}} c_{e,1}\right)\right]}, \quad (5.2)$$

where  $K_i = k_{ad,i}/k_{de,i}$  and  $K_{3,i} = k_{ad,i}/k_{re,1}$  and  $\theta_{e,1}, \theta_{e,2}, c_{e,1} = c_{1,in}$  and  $c_{e,2} = c_{2,in}$ .

Equations (5.1) and (5.2) expressed in terms of the non-dimensional parameters read

$$\theta_{e,1} = \frac{\kappa_2 + \beta(1 + \gamma)}{\kappa_1 + \beta + (1 + \kappa_1)(\kappa_2 + \beta\gamma)}, \quad \theta_{e,2} = \frac{\kappa_1}{\kappa_1 + \beta + (1 + \kappa_1)(\kappa_2 + \beta\gamma)}. \quad (5.3)$$

A single-component isotherm defines a curve when plotting  $\theta_{e,i}$  as a function of  $c_{e,i}$ . Equations (5.1) and (5.2) define the two component isotherms which form a surface when plotting  $\theta_{e,i}$  as a function of  $c_{e,1}$  and  $c_{e,2}$ . These isotherms imply that  $K_i = k_{ad,i}/k_{de,i}$  and  $K_{3,i} = k_{ad,i}/k_{re,1}$  are equilibrium constants that should not vary as the equilibrium concentrations change. In fact  $K_i$  may be obtained from the single component isotherms, while  $K_{3,i} \sim 1/k_{re,1}$  must be obtained from the two component isotherms.

From the LEQUIA data [6] we obtain the parameter values presented in Table 1,  $i = 1, 2$  refers to D4, L2 respectively. Both  $K_i, q_{m,i}$  were calculated from the single component isotherm while  $K_{3,i}$  came from the multicomponent data. However, only three data points were provided for the multicomponent isotherm so these values may not be as reliable as the single component ones. The high values of  $K_i$  indicate that adsorption dominates desorption for both contaminants. The values of  $K_{3,i}$ , between 0.15 and 1.5, demonstrate that replacement is of a similar order to adsorption.

Table 1: Parameters obtained from the equilibrium data of [6].

Parameter	Units	Value	
		$i = 1$	$i = 2$
$q_{m,i}$	kg/kg	0.89	0.56
$K_i$	$\text{m}^3/\text{kg}$	1095	3176
$K_{3,i}$	-	0.15	1.5

Table 2: Optimal value of the adsorption and desorption constants (the only parameter fitted has been  $k_{ad,1}$ ). The different data sets are related to the plots in Figure 3.

Parameter	Units	Value		
		(a)	(b)	(c)
$k_{ad,1}$	$\text{m}^3/(\text{kgs})$	0.057	0.04	0.075
$k_{de,1} (\times 10^{-5})$	1/s	5.20	3.65	6.85
$k_{ad,2}$	$\text{m}^3/(\text{kgs})$	0.57	0.40	0.75
$k_{de,2} (\times 10^{-4})$	1/s	1.80	1.26	2.36
$k_{re,1}$	$\text{m}^3/(\text{kgs})$	0.38	0.267	0.50

Noting that  $k_{de,1} = k_{ad,1}/K_1$ ,  $k_{re,1} = k_{ad,1}/K_{3,1}$ ,  $k_{ad,2} = K_{3,2}k_{re,1}$ , the values of Table 1 allow us to reduce the number of unknown parameters in the model to one. It is convenient to choose the adsorption constant of the first sink term  $k_{ad,1}$  as the fitting parameter, since this determines the time-scale  $\tau$ .

In Figure 3 we compare the numerical results against experimental data after optimising for  $k_{ad,1}$ . The squares represent the L2 breakthrough while circles represent D4. From the data we see that initially both molecules are adsorbed (note to better show the fit we start the time axis when L2 starts to escape). As soon as L2 escapes the concentration rises rapidly such that more L2 leaves the column than enters. This can only occur if D4 is rapidly replacing L2. D4 continues to be adsorbed until the column is saturated. The excellent agreement of the model with the experimental data (with a single fitting parameter) suggests that the model is a good candidate to describe the physical system's behaviour.

The values of  $k_{ad,1}$  determined to provide the fit shown in the figures is presented in Table 2. From this and the equilibrium values of Table 1 we are able to calculate all the other coefficients, i.e. the desorption, adsorption of contaminant 2 and replacement.

In [4] it is stressed that adsorption coefficients should remain approximately constant with respect to concentration and occupied sites. Here we see  $k_{ad,1}$  staying close to the average 0.057 for the three different concentrations. Given the lack of fitting and two component isotherm data this appears to be within acceptable bounds. It is also important to highlight that  $k_{ad,1} < k_{re,1} < k_{ad,2}$  is always satisfied.

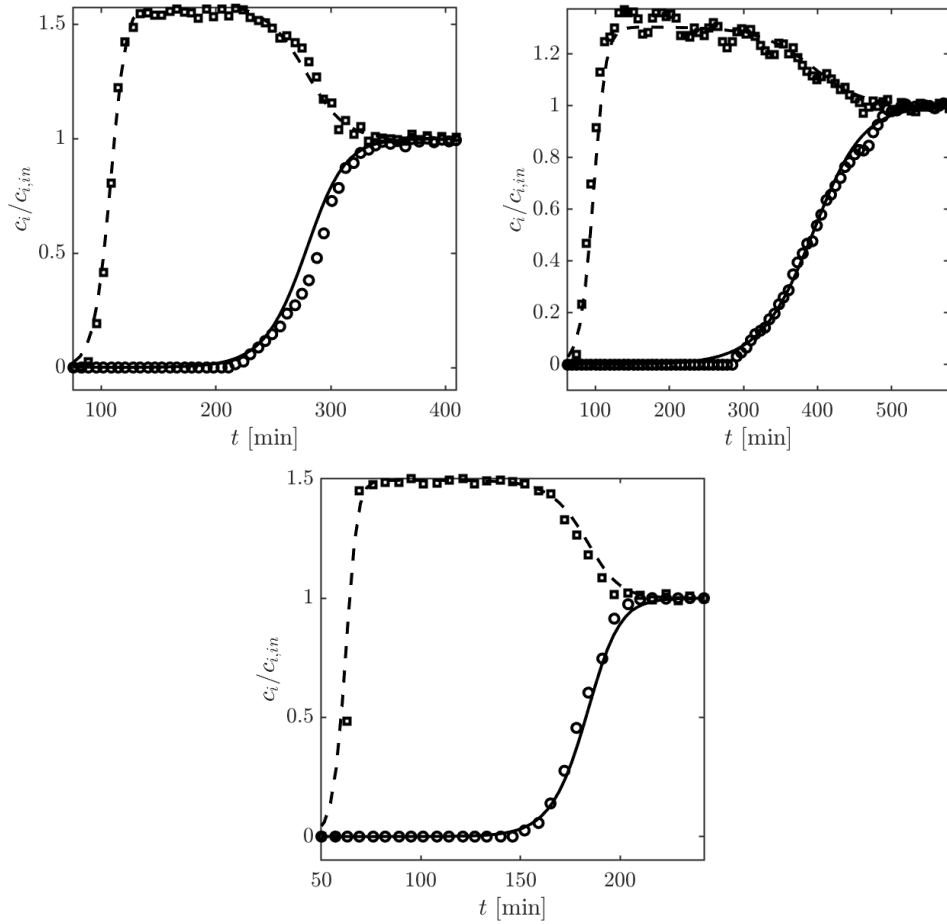


Figure 3: Breakthrough curves for L2 (squares) and D4 (circles). Lines represent the result of the numerical solution. In all cases the flow rate of the carrier fluid is 250mL/min while inlet concentrations of contaminant are: (a)  $c_{1,in} = 0.00302 \text{ kg/m}^3$  and  $c_{2,in} = 0.00307 \text{ kg/m}^3$ ; (b)  $c_{1,in} = 0.00211 \text{ kg/m}^3$  and  $c_{2,in} = 0.00420 \text{ kg/m}^3$ ; (c)  $c_{1,in} = 0.00470 \text{ kg/m}^3$  and  $c_{2,in} = 0.00587 \text{ kg/m}^3$ , where subscript 1 refers to D4 and 2 to L2.



Table 3: Optimised non-dimensional parameter values for the case of L2 and D4 siloxanes with inlet concentrations (a)  $c_{1,in} = 0.00302 \text{ kg/m}^3$  and  $c_{2,in} = 0.00307 \text{ kg/m}^3$ ; (b)  $c_{1,in} = 0.00211 \text{ kg/m}^3$  and  $c_{2,in} = 0.00420 \text{ kg/m}^3$ ; (c)  $c_{1,in} = 0.00470 \text{ kg/m}^3$  and  $c_{2,in} = 0.00587 \text{ kg/m}^3$ .

Parameter	Value		
	(a)	(b)	(c)
$\kappa_1$	0.303	0.432	0.194
$\kappa_2$	0.103	0.075	0.054
$\beta$		6.667	
$\gamma$	0.098	0.050	0.080
$\delta$	0.619	0.317	0.504
Da ( $\times 10^6$ )	3.617	2.531	5.630
Pe $^{-1}$	0.072	0.050	0.095

This suggests that the second component is the first to be adsorbed, since the adsorption of the first component is slow. However, the replacing mechanism is faster than the adsorption of the first component, and hence the first component gradually replaces the second one.

Finally, in Table 3 we present the values of the non-dimensional numbers defined earlier. These can provide key information to guide future work. In particular the value  $\text{Da} = \mathcal{O}(10^{-6})$  indicates we may neglect the  $\partial c/\partial t$  terms. This matches previous work on single contaminants which showed that the concentration rapidly settled to a steady form. Also in keeping with previous work, we find  $\text{Pe}^{-1} = \mathcal{O}(10^{-1})$ , suggesting errors of the order 10% if neglected. In practice it has been shown that the errors are much smaller due to the imposition of the boundary conditions. Although  $\gamma \ll 1$ , in the equations it only appears in the product  $\gamma\beta > 0.3$ , so clearly should be retained.

## 6 Further work

In this report, we show how competitive adsorption can be described by extending the single contaminant model developed by Myers *et al.* [4]. The resulting system consists of 2 equations for each contaminant, one describing the transport along the column and one focusing on the adsorption, desorption and competition mechanisms. Due to the interaction between the contaminants, the travelling wave approach failed and needs some rethinking before an analytical solution can be found. The numerical solutions gave promising results as they show that the model is able to capture the experimental behaviour. In future work we intend extend the work even further. Starting with the two component model we need to bring in more information, such as from the isotherms, and carry out less fitting. With a better understanding of the

two component system a key goal is to then move on to more contaminants, which is typically the case with flue gases.

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