# Adsorption of multiple contaminants from a fluid stream

*MISG2023*

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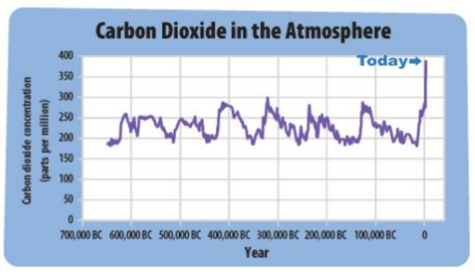
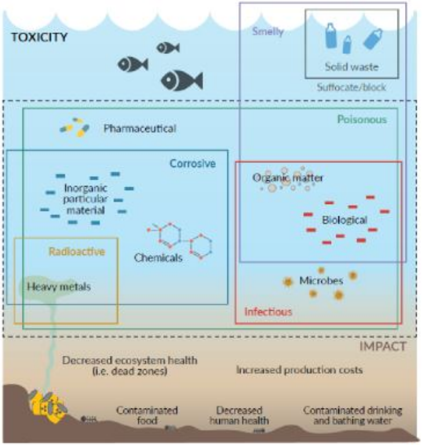
# CARBON CAPTURE

**Global warming:** the increase in Earth's average surface temperature due to rising levels of greenhouse gases.

**Climate change:** a long-term change in the Earth's climate, or of a region on Earth.

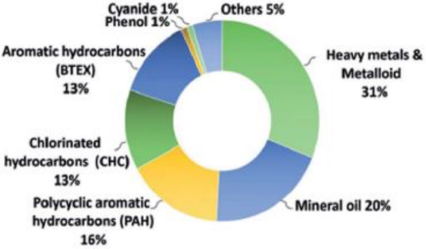


# WATER TREATMENT



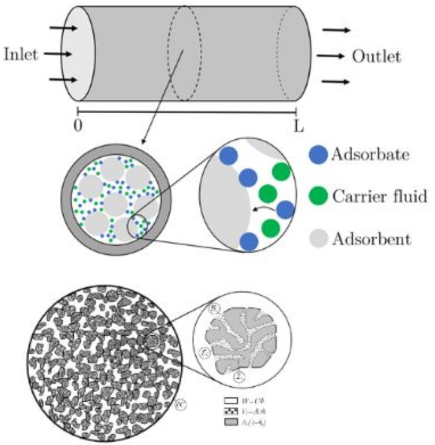

Source: Adapted from Corcoran et al. (2010, Fig. 5, p. 21)

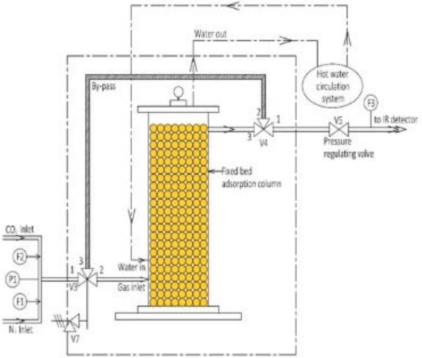
- Pharmaceuticals
- Heavy Metals
- Fluoride
- Dyes
- Pharmaceutical
- VOCs, SOCs and suspended particles




Source: Norrrahim et al. (2021, Fig. 1, p. 7349)

# Contaminant Removal by sorption



# One Contaminant (existing model)

Fluid Variables:

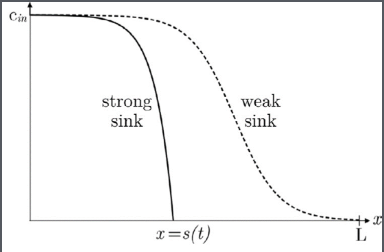
$c_i(x, t)$ is the concentration of free contaminant $i$ in the carrier fluid.

Adsorbent:

$q_i(x, t)$ is the mass of adsorbed contaminant $i$.

$\theta_i(x, t) = q_i(x, t)/q_{m,i}$ is the proportion of sites occupied by contaminant $i$.

Typical concentration profiles through the column



# Governing Equations

Advection-diffusion equations:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - \frac{q_m \rho_b}{\phi}\frac{\partial \theta}{\partial t}$$

Kinetic equations:

$$\frac{\partial \theta}{\partial t} = k_{ad} c \left(1 - \theta\right) - k_{de}\theta$$

Boundary and initial conditions

$$uc_{in} = uc - D\frac{\partial c}{\partial x}, \qquad x = 0$$

$$\frac{\partial c}{\partial x} = 0, \qquad x = L$$

$$c = \theta = 0, \qquad t = 0$$

# Curve fitting for one contaminant (no interaction)

Travelling Wave solutions

$$\frac{c(l,t)}{c_{in}} = \frac{1}{1+\exp\left(k_{ad}c_{in}(t_{1/2}-t)\right)}$$

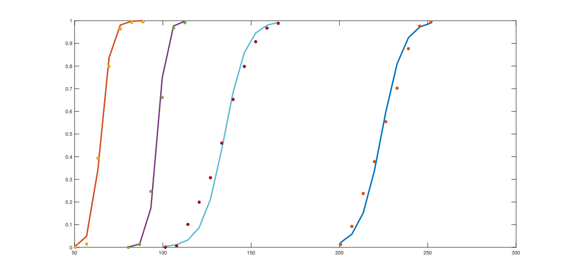
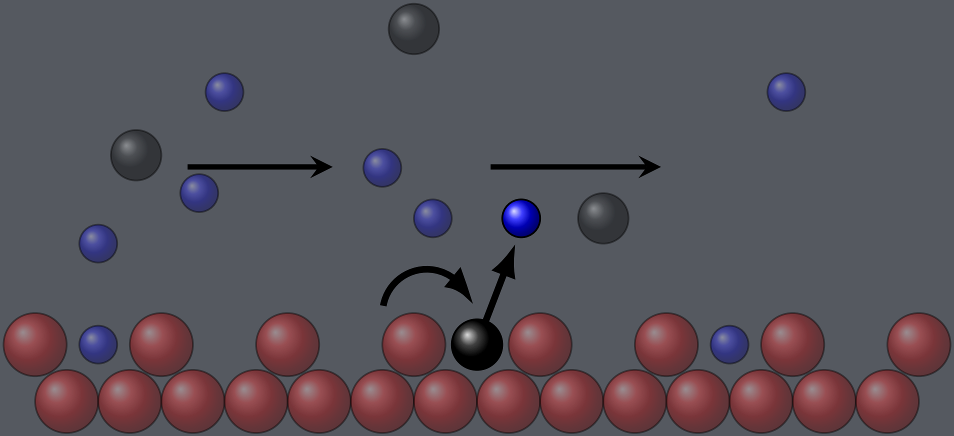



**Figure 1:** $k_{ad} = 4.7839, 7.9604, 4.4649, 8.6349 \times 10^{-5}$

# Two Contaminant



# Chemical Reactions

Reaction 1: Contaminant $c_1$ attaches to adsorbent $A$ but can also slowly desorb

$$c_1 + A \underset{k_{de,1}}{\overset{k_{ad,1}}{\rightleftharpoons}} c_1A \quad , \qquad r_1 = k_{ad,1} c_1 \left(1 - \theta_1 - \theta_2\right) - k_{de,1}\theta_1$$

Reaction 2: Contaminant $c_2$ attaches to A and slowly desorbs

$$c_2 + A \underset{k_{de,2}}{\overset{k_{ad,2}}{\rightleftharpoons}} c_2A \quad , \qquad r_2 = k_{ad,2} c_2 \left(1 - \theta_1 - \theta_2\right) - k_{de,2}\theta_2$$

Reaction 3: Contaminant $c_1$ knocks off adsorbed $c_2$ and $c_2$ does the same to $c_1$

$$c_1 + c_2A \underset{k_{ko,2}}{\overset{k_{ko,1}}{\rightleftharpoons}} c_1A + c_2 \quad , \qquad r_3 = k_{ko,1} c_1 \theta_2 - k_{ko,2} c_2 \theta_1$$

# Governing Equations

Advection-diffusion equations:

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} = D\frac{\partial^2 c_i}{\partial x^2} - \frac{q_{i,m}\rho_b}{\phi}\frac{\partial \theta_i}{\partial t}$$

Kinetic equations:

$$\frac{\partial \theta_i}{\partial t} = \underbrace{k_{ad,i}c_i\left(1-\theta_1-\theta_2\right) - k_{de,i}\theta_i}_{Individual} \underbrace{+k_{ko,i}c_i\theta_j - k_{ko,j}c_j\theta_i}_{Interaction}$$

Boundary and initial conditions

$$uc_{i,in} = uc_i - D\frac{\partial c_i}{\partial x}\,, \qquad x = 0$$

$$\frac{\partial c_i}{\partial x} = 0\,, \qquad x = L$$

$$c_i = \theta_i = 0\,, \qquad t = 0$$

# Non-dimensional formulation

We scale as follows:

$$c_i \sim c_{i,in}\,, \quad t \sim \tau = \frac{1}{k_{ad,1}c_{1,in}}\,, \quad x \sim \mathcal{L} = \frac{c_{1,in}\tau u \phi}{q_{i,m}\rho_b}$$

$$\begin{aligned}
\mathrm{Da}\frac{\partial \bar{c}_1}{\partial \bar{t}} &= -\frac{\partial \bar{c}_1}{\partial \bar{x}} + \mathrm{Pe}^{-1}\frac{\partial^2 \bar{c}_1}{\partial \bar{x}^2} - \frac{\partial \theta_1}{\partial \bar{t}}\,,\\
\mathrm{Da}\frac{\partial \bar{c}_2}{\partial \bar{t}} &= -\frac{\partial \bar{c}_2}{\partial \bar{x}} + \mathrm{Pe}^{-1}\frac{\partial^2 \bar{c}_2}{\partial \bar{x}^2} - \delta\frac{\partial \theta_2}{\partial \bar{t}}\,,\\
\frac{\partial \theta_1}{\partial \bar{t}} &= \bar{c}_1\left(1-\theta_1-\theta_2\right) - k_1\theta_1 + \beta_1\bar{c}_1\theta_2 - \beta_2\bar{c}_2\theta_1\,,\\
\frac{\partial \theta_2}{\partial \bar{t}} &= \zeta\left[\bar{c}_2\left(1-\theta_1-\theta_2\right) - k_2\theta_2\right] - \beta_1\bar{c}_1\theta_2 + \beta_2\bar{c}_2\theta_1\,.
\end{aligned}$$

# Non-dimensional Parameters

$$\mathrm{Da} = \frac{u\mathcal{L}}{\tau}, \quad \mathrm{Pe}^{-1} = \frac{D}{\mathcal{L}u}, \quad \delta = \frac{q_{2,m}c_{1,in}}{q_{1,m}c_{2,in}},$$

$$k_i = \frac{k_{de,i}}{k_{ad,i}c_{i,in}}, \quad \beta_i = \frac{k_{ko,i}c_{i,in}}{k_{ad,1}c_{1,in}}, \quad \zeta = \frac{k_{ad,2}c_{2,in}}{k_{ad,1}c_{1,in}}$$

At equilibrium we have $c_i \to 1$ and $\theta_i \to \theta_{i,e}$, where

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 + k_1 + \beta_2 & 1 - \beta_1 \\ \zeta - \beta_2 & \zeta + \zeta k_2 + \beta_1 \end{bmatrix} \begin{bmatrix} \theta_{1,e} \\ \theta_{2,e} \end{bmatrix}$$

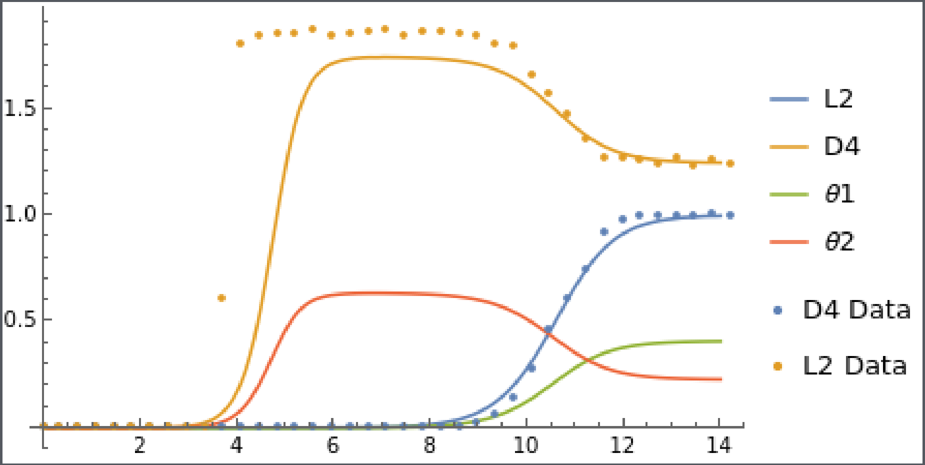
# Numerical Solution for Multicontaminant Problem

Mathematica (Sorry John) - NDSolveValue[*eqns*, *y*[*x*], {*x*, *xmin*, *xmax*}] gives solutions for y[x] rather than for the function y itself.

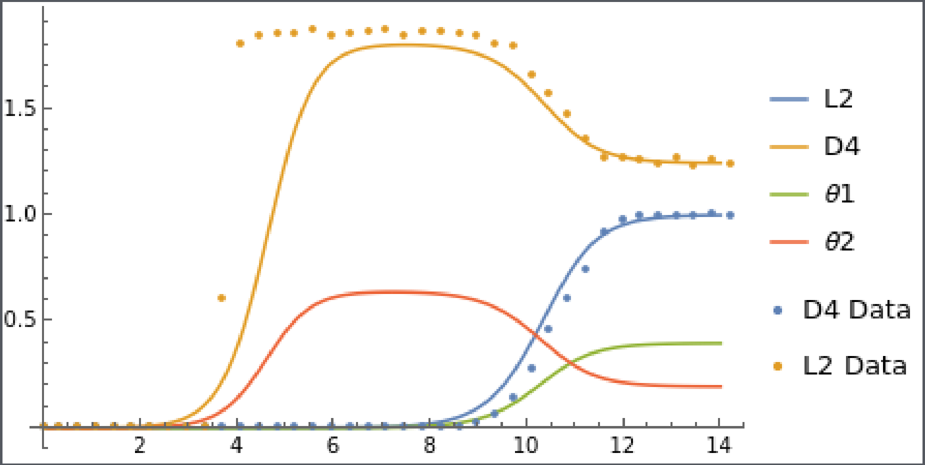
NDSolveValue - NDSolveValue typically solves differential equations by going through several different stages depending on the type of equations. With Method->$s_1$->$m_1$,$s_2$->$m_2$,..., stage $s_i$ is handled by method $m_i$. The actual stages used and their order are determined by NDSolve, based on the problem to solve.

Method of Lines - The numerical method of lines is a technique for solving partial differential equations by discretising in all but one dimension and then integrating the semi-discrete problem as a system of ODEs or DAEs.

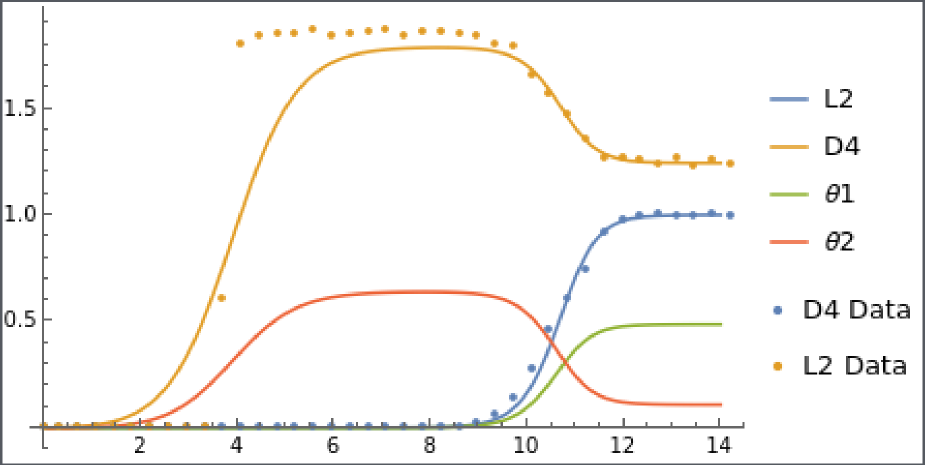
Spatial Discretisation - TensorProductGrid 1001 points

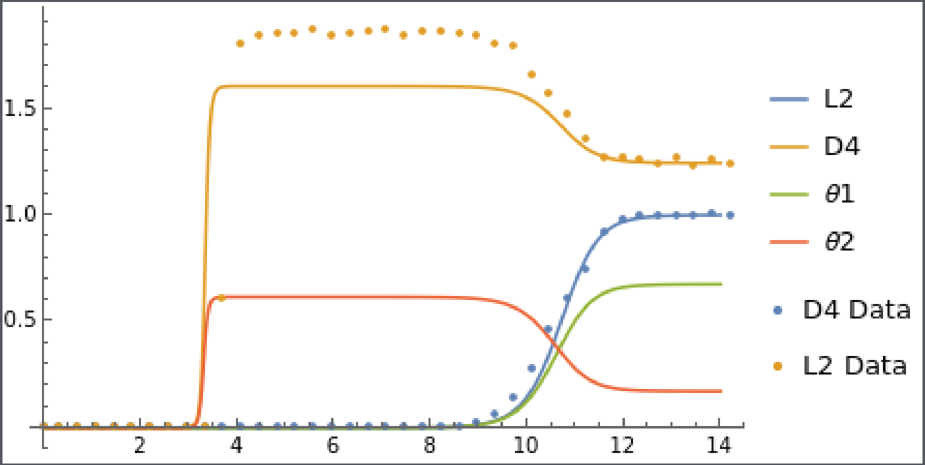


1.5
1.0
0.5
2
4
6
8
10
12
14
L2
D4
θ1
θ2
D4 Data
L2 Data



1.5
1.0
0.5
2
4
6
8
10
12
14
L2
D4
θ1
θ2
D4 Data
L2 Data

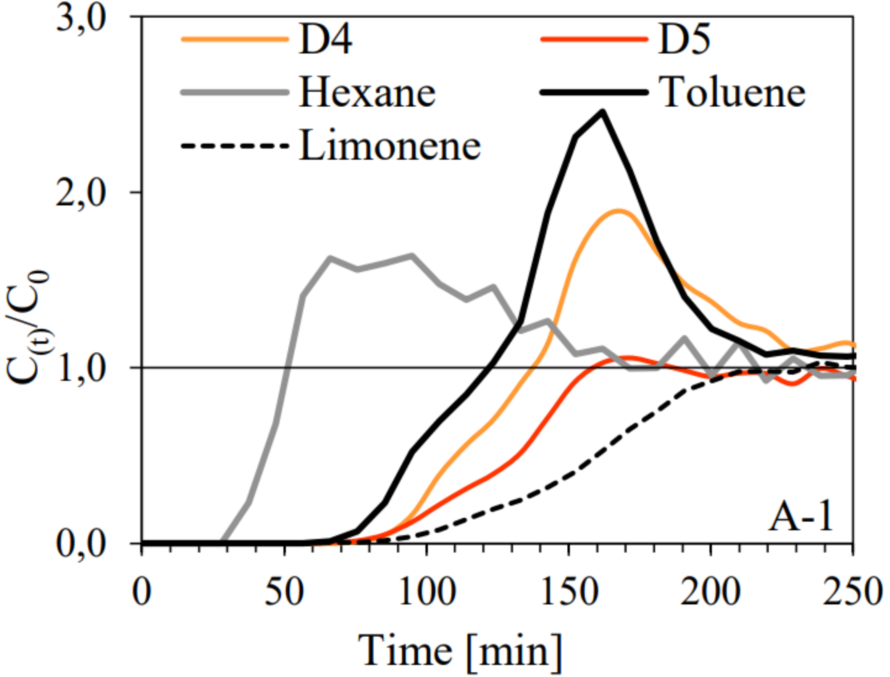

1.5
1.0
0.5
2
4
6
8
10
12
14
L2
D4
θ1
θ2
D4 Data
L2 Data



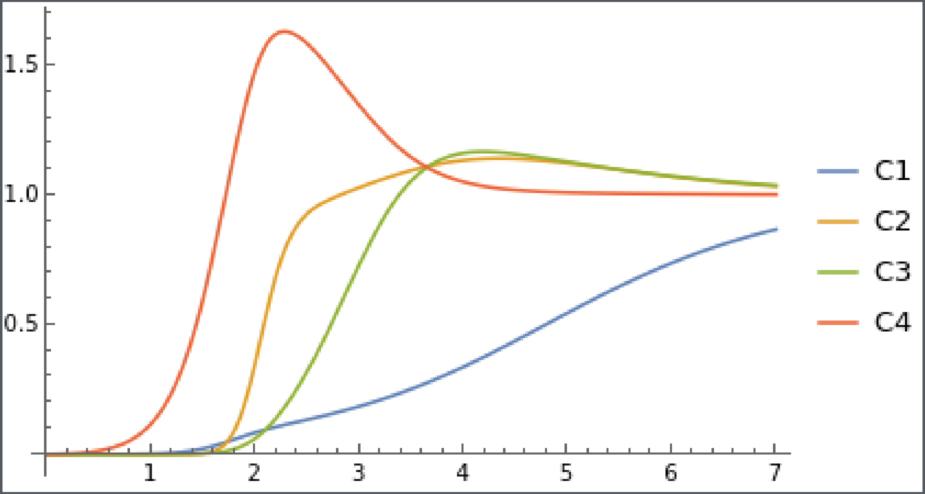
1.5
1.0
0.5
2
4
6
8
10
12
14
L2
D4
θ1
θ2
D4 Data
L2 Data

# END GOAL

n-contaminant problem



D4
D5
Hexane
Toluene
Limonene
A-1
3,0
2,0
1,0
0,0
0
50
100
150
200
250
$C_{(t)}/C_0$
Time [min]


1.5
1.0
0.5
1
2
3
4
5
6
7
C1
C2
C3
C4

# Final thoughts

The proposed model seems to capture the competing nature of the 2 components

Proper numerics and data fitting needs to be done.

n-contaminant model appears to be viable with further investigation needed.