Adsorption of multiple contaminants from a fluid stream

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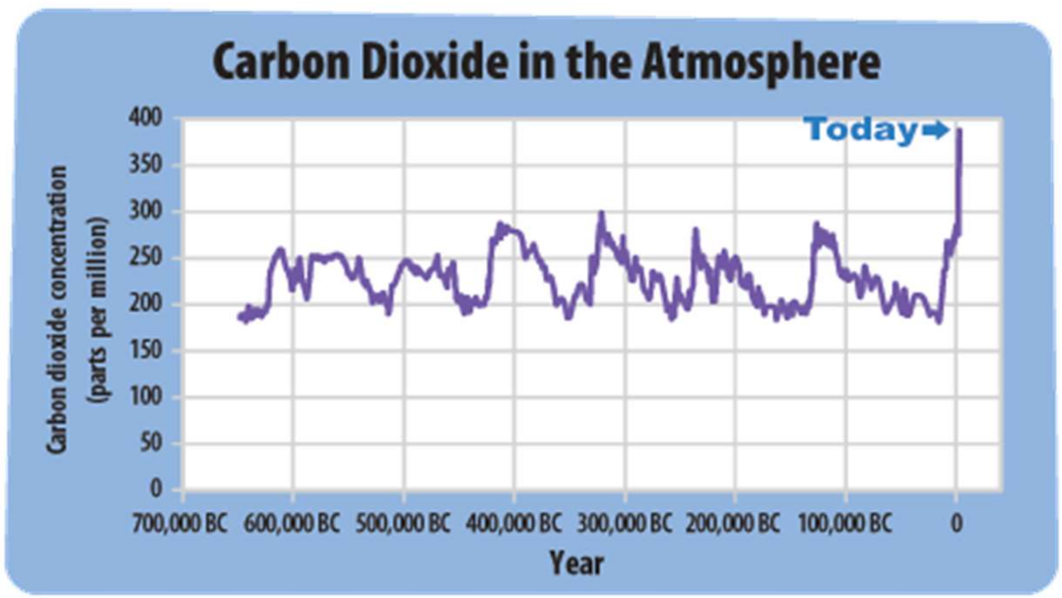
MOTIVATION

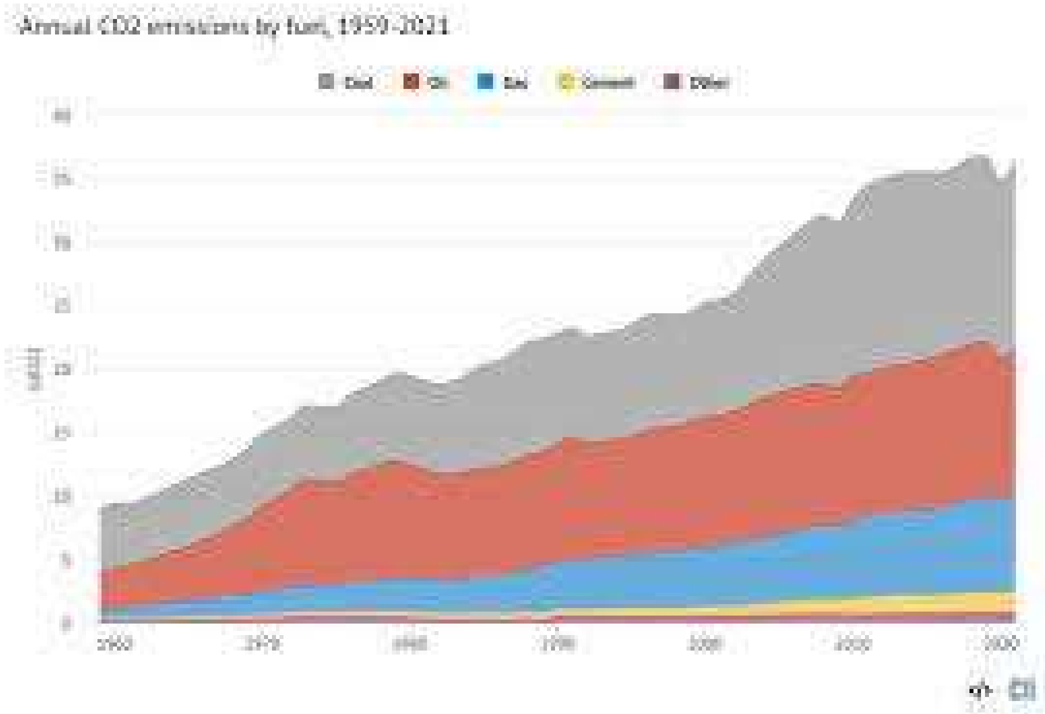
CARBON CAPTURE

- **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.

Likelihood of more extreme events: more powerful storms, heat waves, flooding, etc.



CARBON CAPTURE



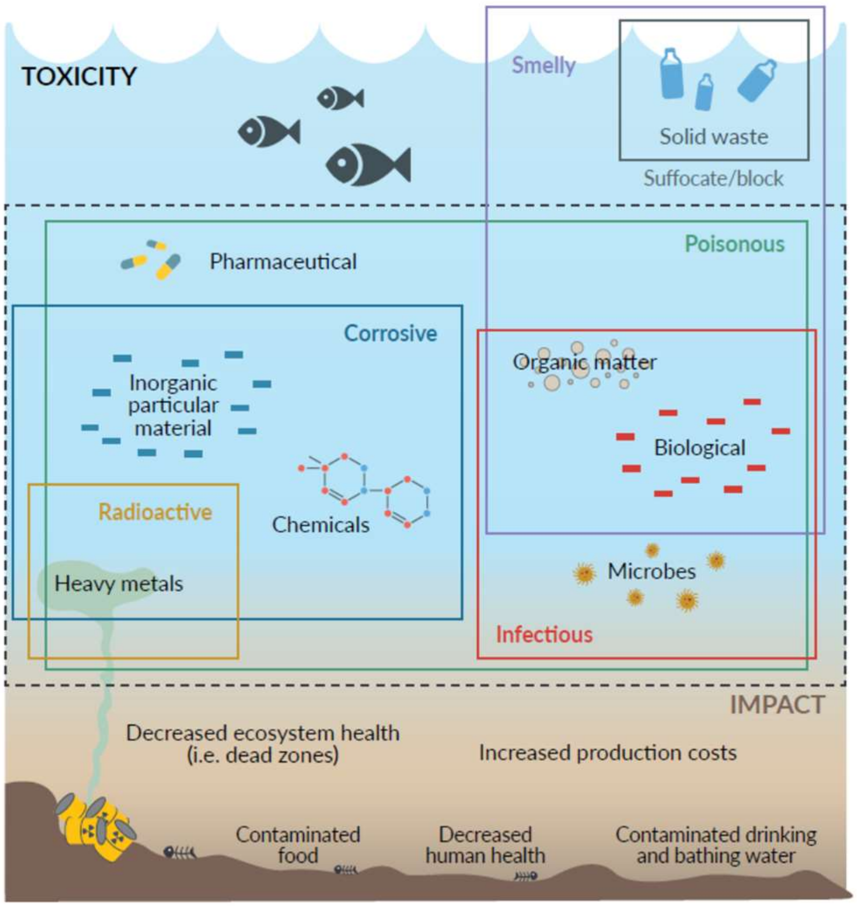
Source: carbonbrief.org

Paris Agreement at the COP21 conference in 2015/Glasgow COP26:

- **Keep the global temperature rise below 2°C above pre-industrial levels**
- **Pursue efforts to limit the temperature increase even further to 1.5°C**

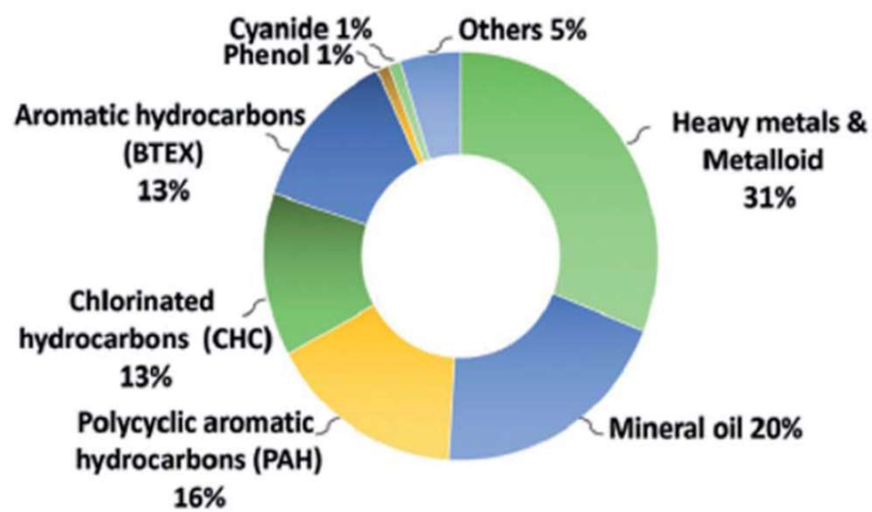
The IPCC, the international body that issues comprehensive reports on climate change, has estimated that the world will need to be removing an average of 10 gigatons of CO_2 (10 billion tons) a year from the atmosphere by midcentury.

WATER TREATMENT



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

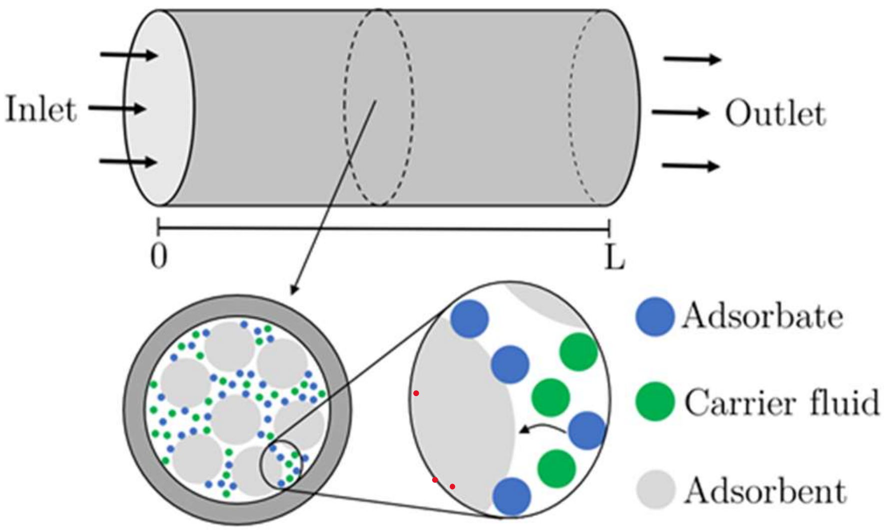
- Pharmaceuticals
- Heavy Metals
- Fluoride
- Dyes
- Pharmaceutical
- VOCs, SOCs and suspended particles

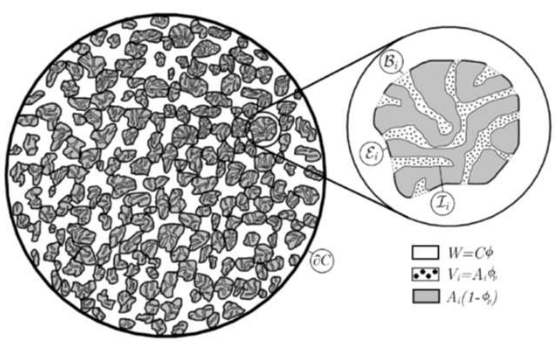


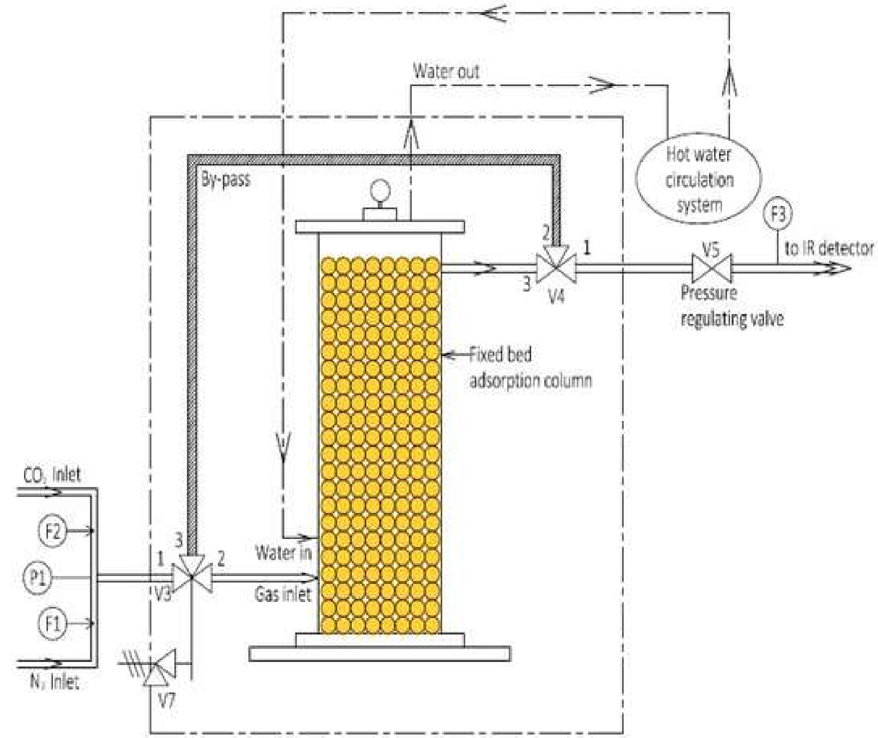
Source: Norrrahim et al. (2021, Fig. 1, p. 7349)

ADSORPTION

CONTAMINANT REMOVAL BY SORPTION

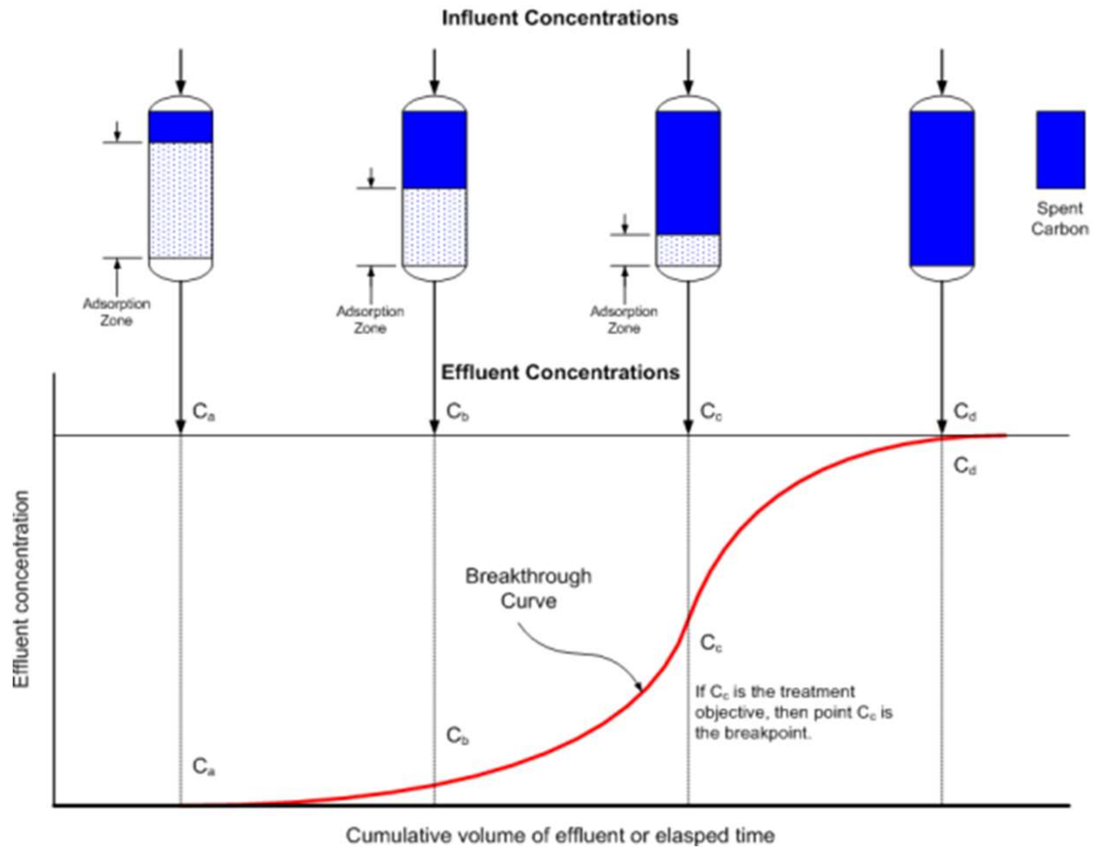






Breakthrough curve

Concentration measured at column outlet



THE BREAKTHROUGH CURVE

The **BREAKTHROUGH CURVE** is the curve that accounts for the temporal evolution of the concentration of the contaminant at the outlet of the column, i.e. $c(L,t)$ (or normalized as $c(L,t)/c_{in}$, where c_{in} is the inlet concentration).

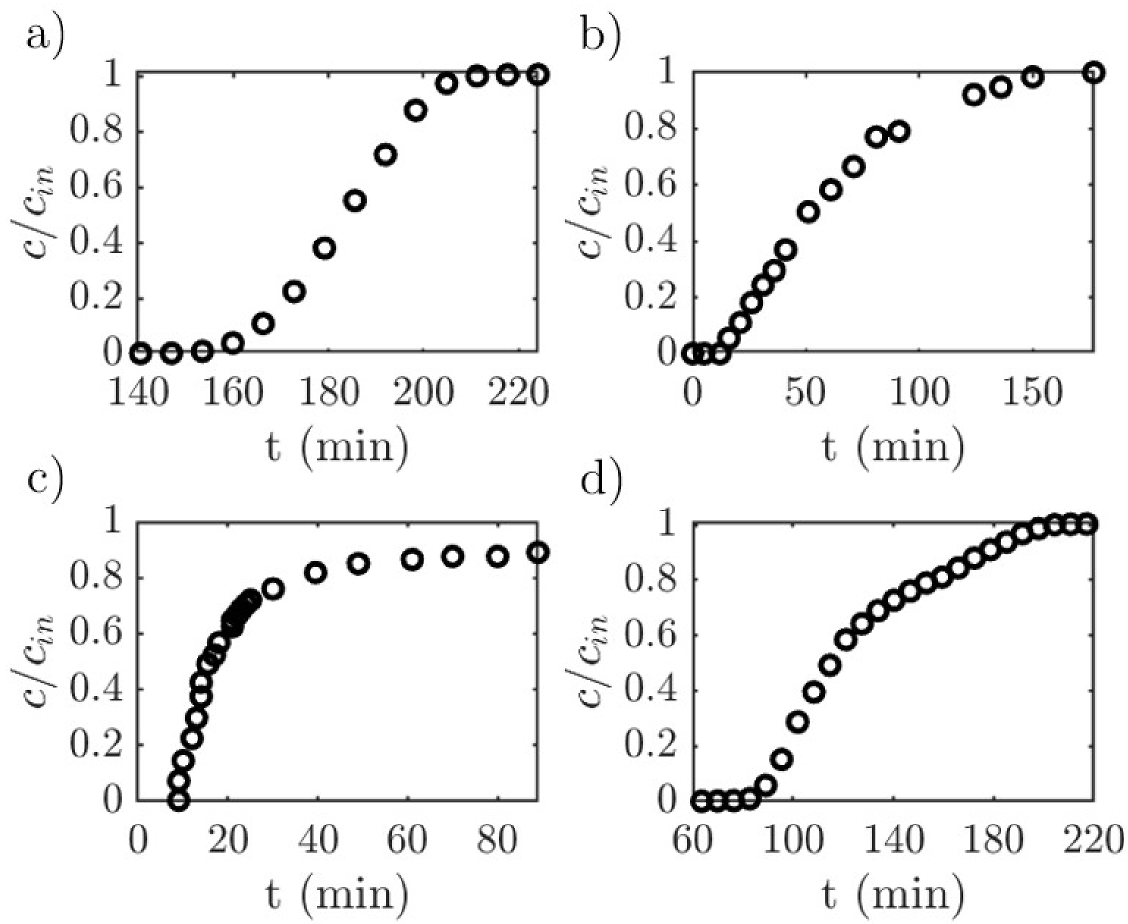
Breakthrough curve types:

a) **Symmetric (S)** → toluene on activated carbon,

b) **Asymmetric rapid decay (ARD)** → Cr^{3+} on NaX zeolite,

c) **Asymmetric slow decay (ASD)** → amoxicillin on activated carbon,

d) **Asymmetric piecewise (APW)** → toluene on activated carbon.



ADVECTION-DIFFUSION EQUATION

Mass balance for mass of contaminant in a cross-section

$$\frac{\partial m_c}{\partial t} + \frac{\partial}{\partial x}\left(u m_c - D\frac{\partial m_c}{\partial x}\right) = -\frac{\partial m_{ad}}{\partial t}$$

$m_c = \epsilon A c \qquad m_{at} = M_{at}/L,$

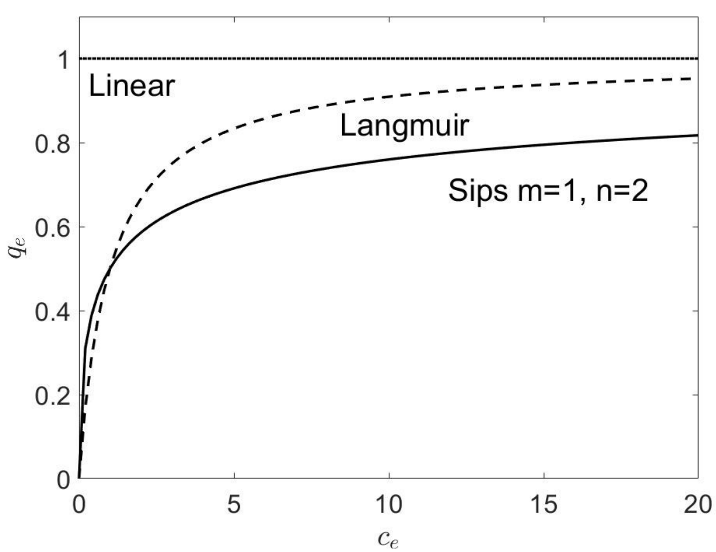
$$\frac{\partial}{\partial t}(\epsilon A c) + \frac{\partial}{\partial x}(u \epsilon A c) = \frac{\partial}{\partial x}\left(D\frac{\partial}{\partial x}(\epsilon A c)\right) - m_{at}\frac{\partial q}{\partial t}$$

$\rho_b = M_{at}/(AL)$

$$\frac{\partial}{\partial t}(\epsilon c) + \frac{\partial}{\partial x}(u \epsilon c) = \frac{\partial}{\partial x}\left(D\frac{\partial}{\partial x}(\epsilon c)\right) - \rho_b\frac{\partial q}{\partial t}$$

SINK MODELS

$$\frac{\partial q}{\partial t} = Q(c, q)$$



Langmuir sink

$$Q(c, q) = k_{ad} c (q_m - q) - k_{de} q$$

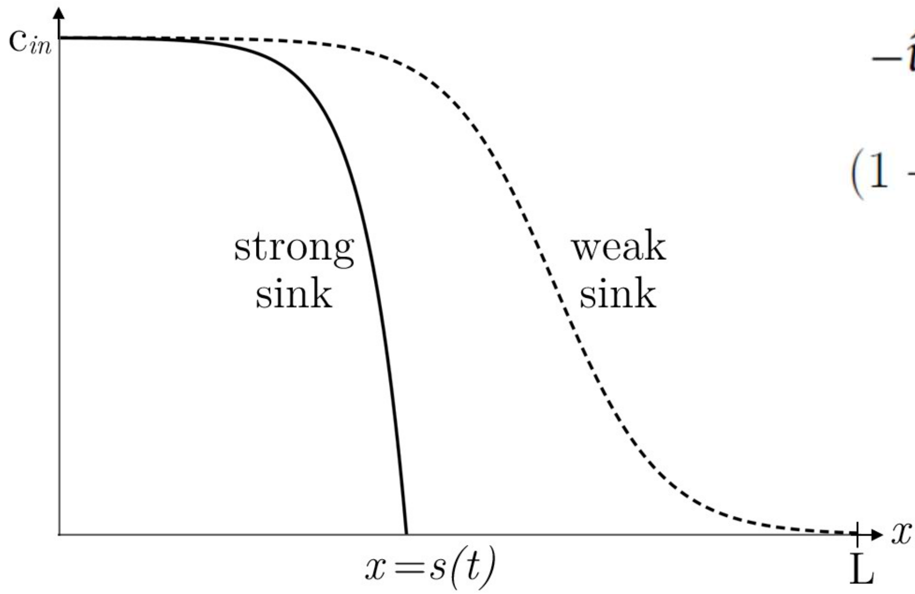
Isotherm = equilibrium information

Langmuir isotherm

$$q_e = \frac{q_m K_L c_e}{1 + K_L c_e}$$

TRAVELLING WAVE

Non-dimensionalise and $\eta = \hat{x} - \hat{s}(\hat{t})$



Langmuir sink

$$-\hat{v}G' = F(1-G) - \delta_3\ G\,.$$

$$(1-\hat{v}\delta_1)F' = \delta_2 F'' + \hat{v}G'$$

$$F = F' = G = 0$$

$$\delta_1, \delta_2 \ll 1$$

$$F = \frac{1}{1 + B\exp(\eta/\hat{v})}$$

F=0??

=> Weak sink

$$\frac{c}{c_{in}} = \frac{1}{1+\exp\left[k_{ad}c_{in}((x-L)/v + (t_{1/2}-t))\right]} = (1+\delta_3)\frac{q}{q_m}$$

COMPARISON WITH DATA

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

Works great – for some cases

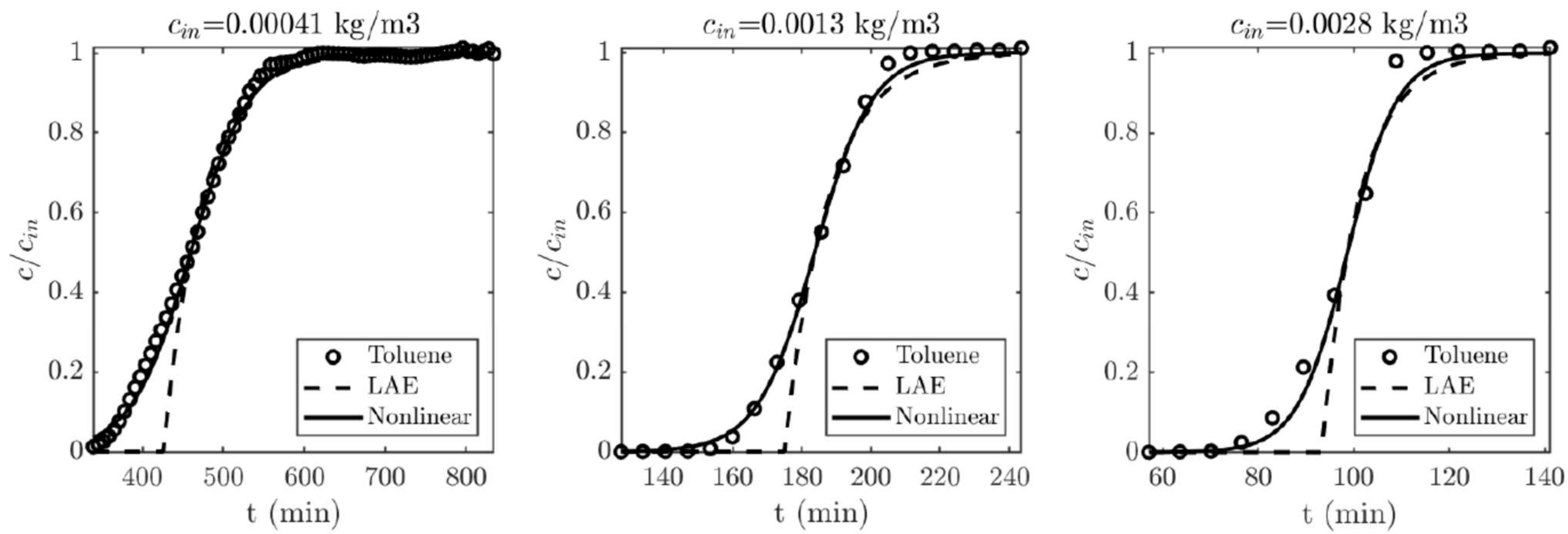


Figure 2: Comparison of models for toluene adsorption on steam activated carbon. Solid line nonlinear adsorption equation (47), dashed line linear adsorption equation (41), circles represent the data points.

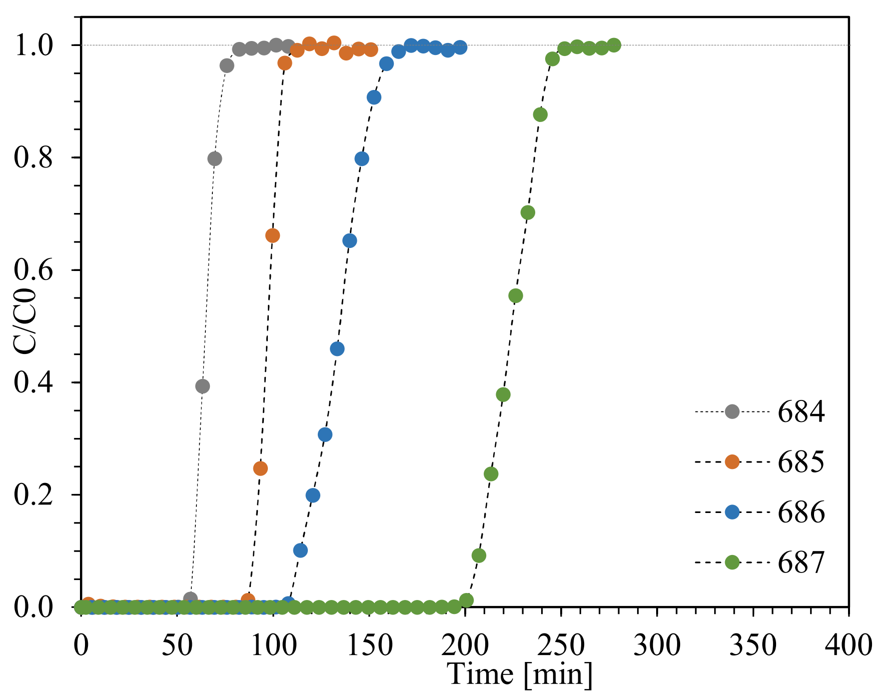
BUT IN REALITY ...

Emissions aren’t just one contaminant, they are an unpleasant combination

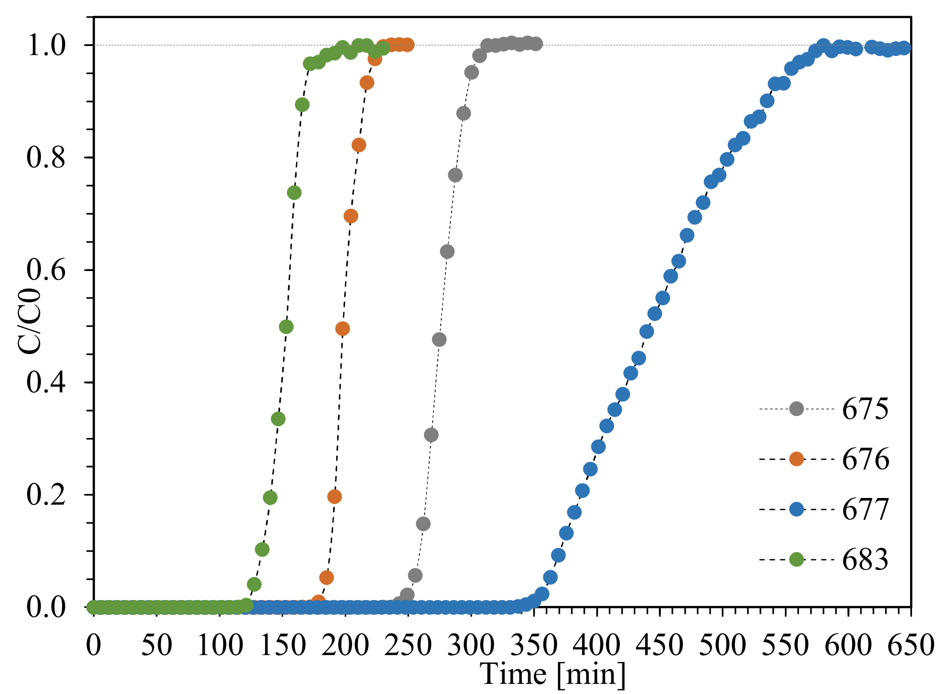
A rather unpleasant chimney emission, taken from https://www.tradeindia.com/products/stack-chimney-emission-and-flue-g treatment-from-aeolus-c4994396.html

TWO COMPONENT

L2 (2 atoms of Si)

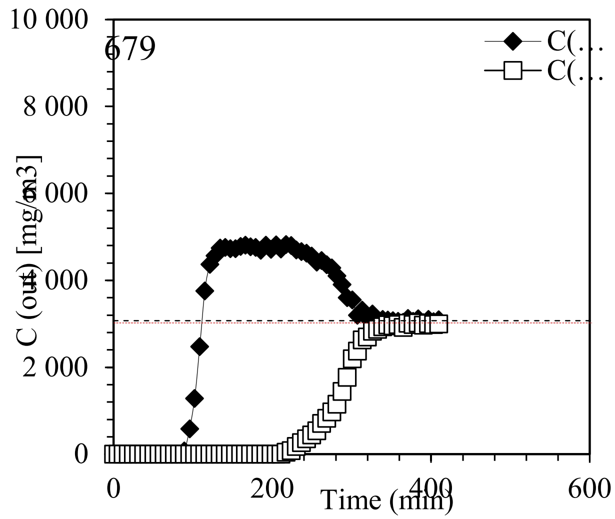


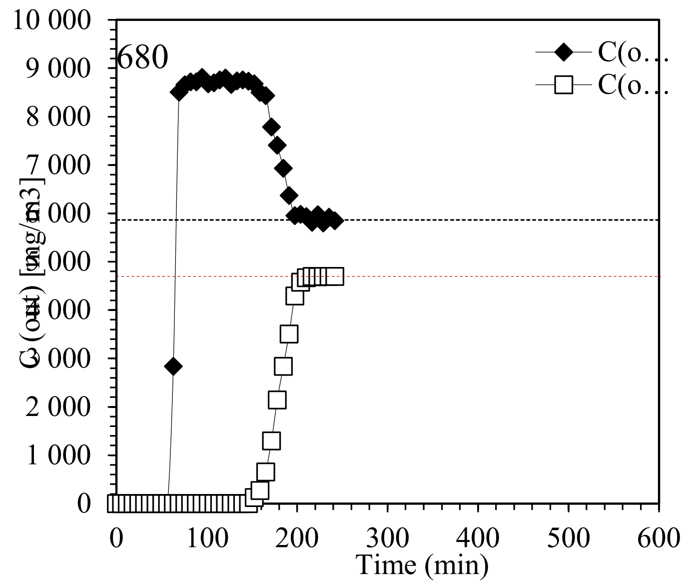
D4 (4 atoms of Si)

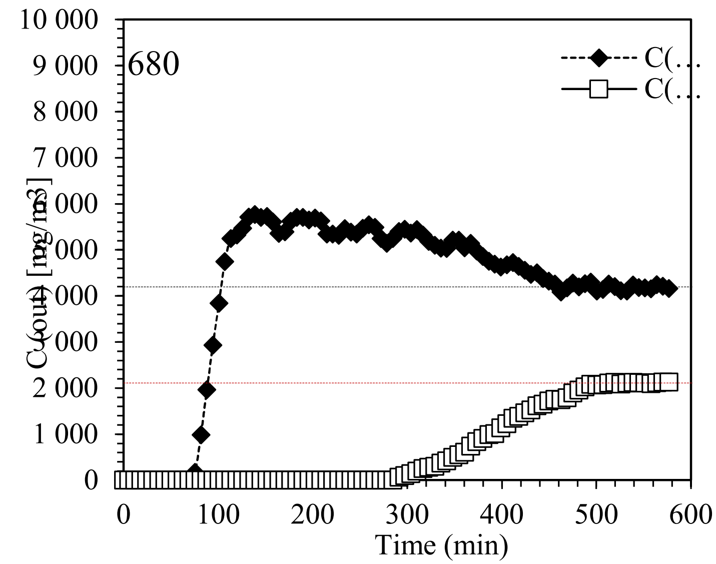


L2, D4 are volatile methyl silicone compounds – coming from personal care products (shampoo, body lotions etc)

COMPETITIVE ADSORPTION

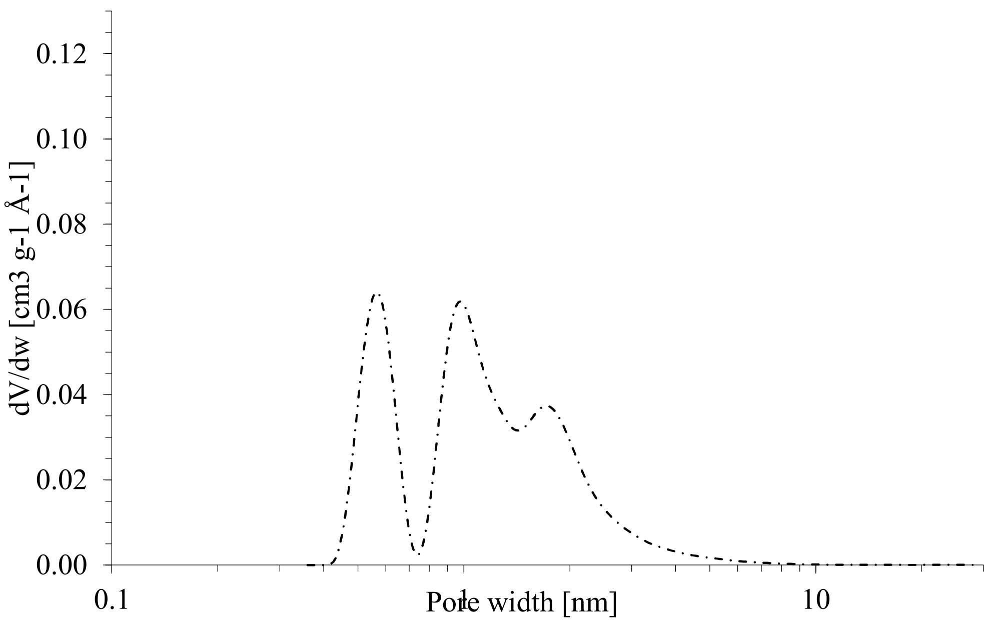


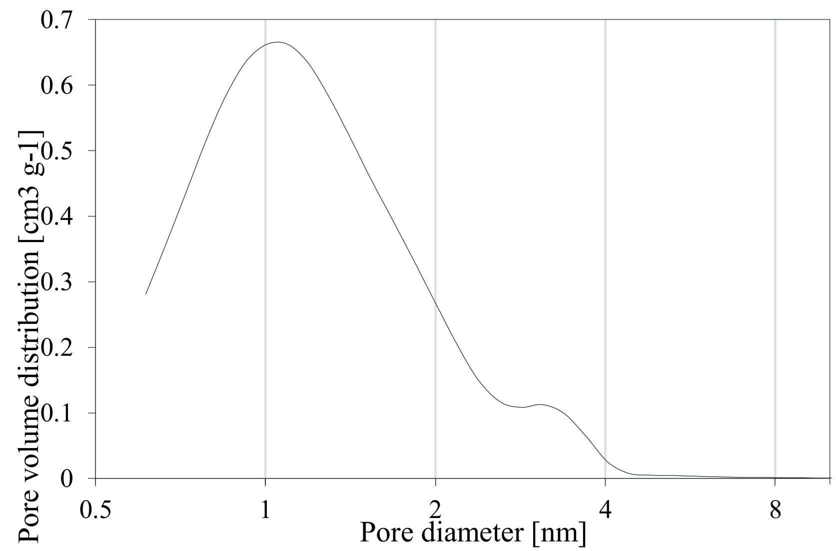


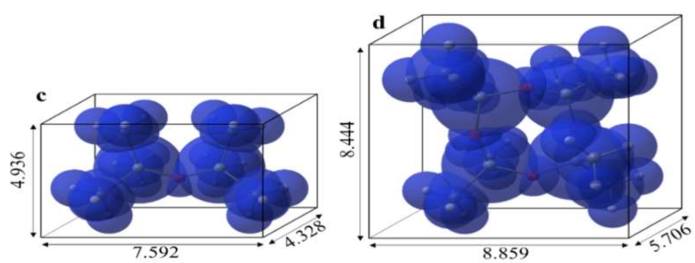


L2 rapidly adsorbed but then displaced by D4

ALBA MADE ME INCLUDE THIS

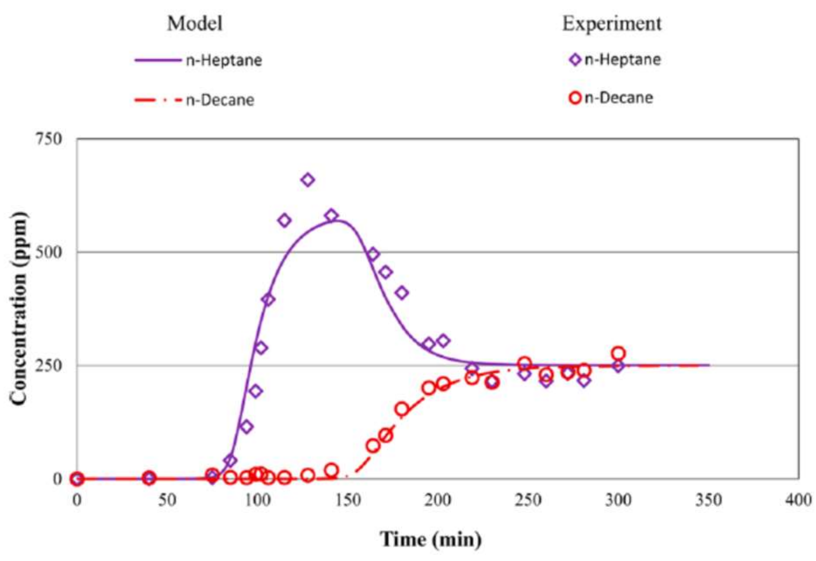




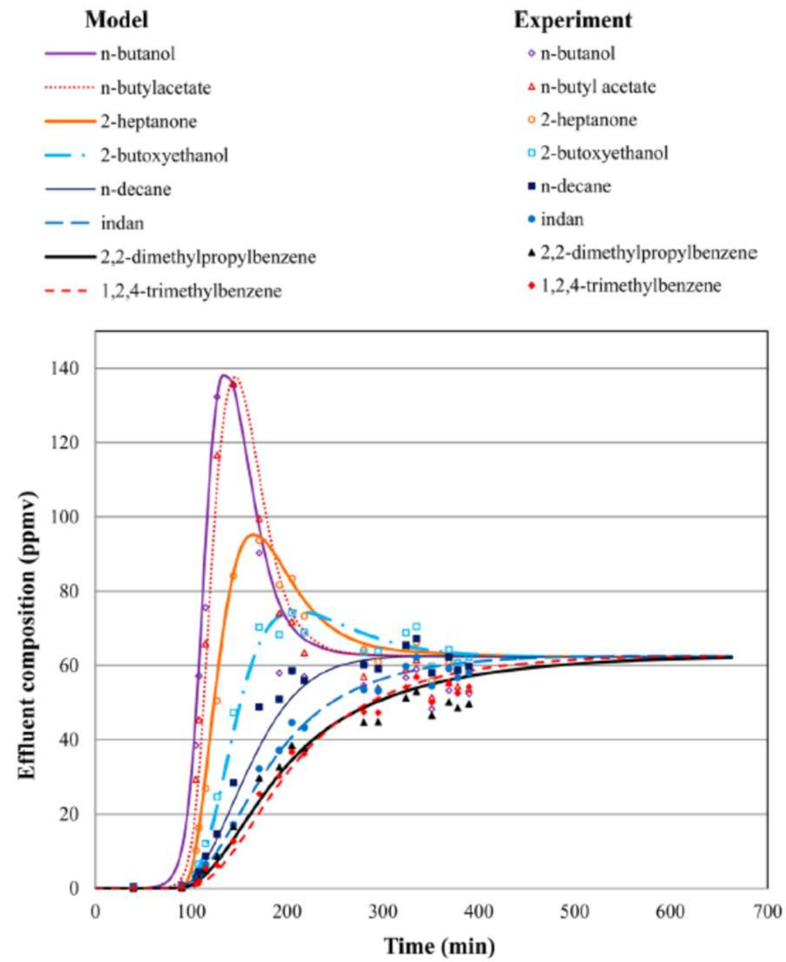


angstroms + 1.2 Å x2 van der Waals

ADSORPTION OF EXHAUST GAS



(a)

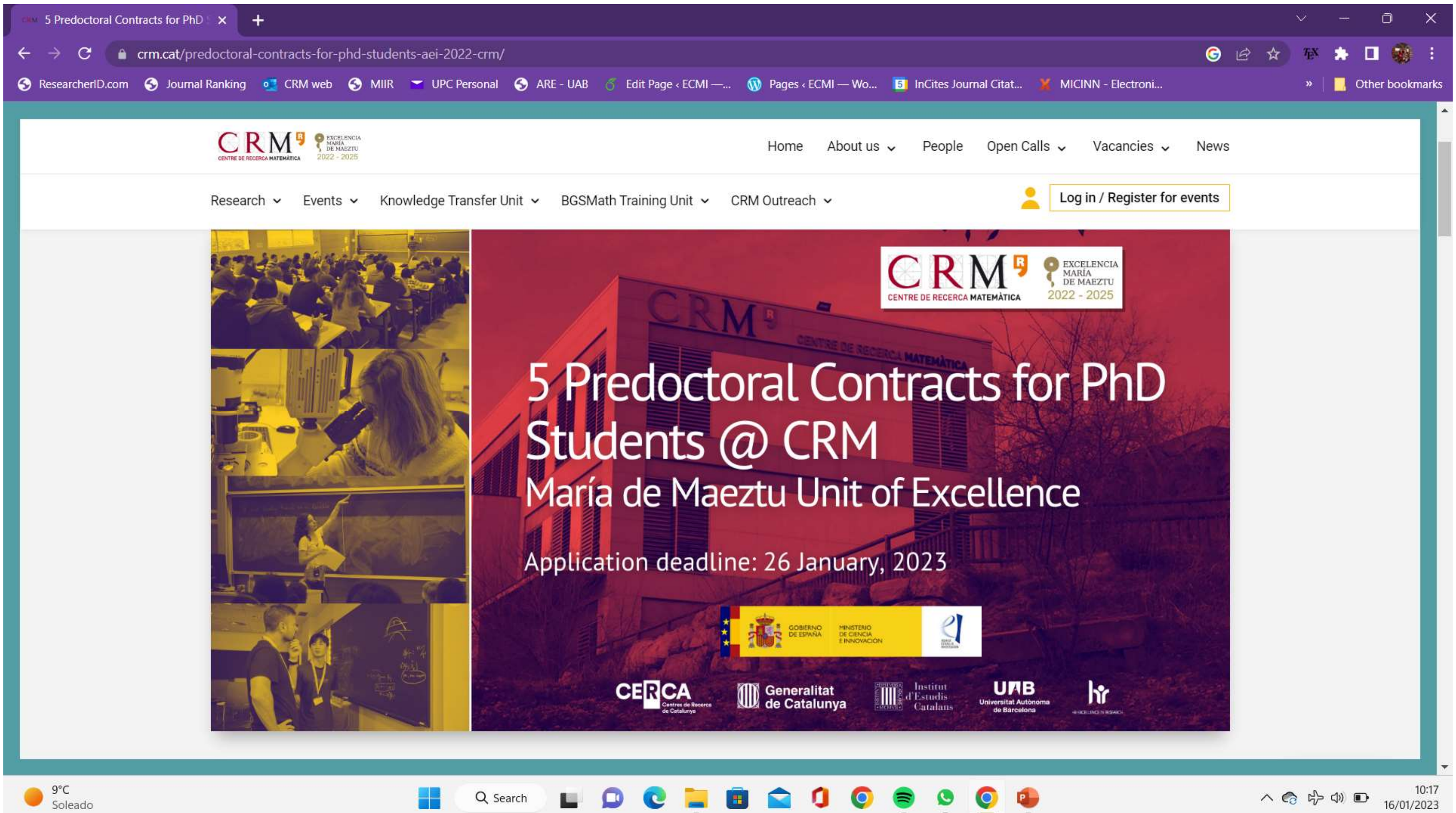


Numerical solutions for 2 and 8 components – Tefera et el 2014

GOALS FOR MISG

1. Develop model for two component adsorption – extend previous work (c.f. population modelling)
2. Develop approximate and or TW solutions (if possible)
3. Develop numerical solutions
4. Verify against experimental data (get Alba to do some work)
5. Extend to n >2 components
6. Solve however possible
7. Make the world a little better

AND FINALLY ...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