Carbon Capture Using Adsorption

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Problem Statement

- **Carbon dioxide levels have risen dramatically in recent decades, going from 280ppm to over 400**
- **This rise is much larger than those owing to natural fluctuations - caused by human burning of fossil fuels for electricty and transport**
- **Has lead to significant climate change, and if this pattern continues there may be catastrophic consequences**
- **Many people rely on fossil fuels, and so it is easier to extract the greenhouse gases than to stop creating them**
- **One option to achieve such a goal is Carbon Capture and Storage, which needs to be modelled**

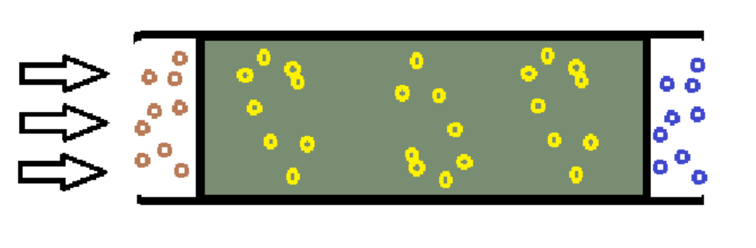
Introduction

- **Carbon Capture and Storage is a technology that can capture up to 90% of carbon dioxide (CO_2) emissions produced from the use of fossil fuel.**
- **Capture methods include chemical and physical adsorption**
- **In the case of physical adsorption, the gas flows over or through an absorptive material. A specific case could be thatan adsorbent fills a pipe and gas is allowed into the pipe, and then some gas molecules will attach to the material.**

Introduction (continued)

- **Adsorbents include metal-organic framework structures (MOFs), microporous and mesoporous materials such as zeolite or dolomite, carbon-based solids and others**
- **Our analysis include carbon-based solids such as Activated Carbon which have been proven to be one of the most effective and economically friendly absorbents in industry.**

Carbon Capture In A Fixed Bed



Governing Equations

$$\epsilon\frac{\partial C_j}{\partial t} + \nabla \cdot (C_j \boldsymbol{u}) = \epsilon D \nabla^2 C_j - (1-\epsilon)\rho_p \frac{\partial q_j}{\partial t} \tag{1}$$

$$\frac{\partial q_j}{\partial t} = K_j^L (q_j^* - q_j) \tag{2}$$

$$q_j^* = \frac{q_j^m K_j^{eq} P_j}{\left[1 + \left(K_j^{eq} P_j\right)^n\right]^{1/n}} \tag{3}$$

$$K_j^{eq} = K_j^0 e^{-\Delta H / R T_g} \tag{4}$$

$$P_j = C_j R T_g \tag{5}$$

Neglected Equations

$$-\frac{\partial P}{\partial x} = 150\frac{\mu_g(1-\epsilon)^2}{\epsilon^2 d_p^2}u + 1.75\frac{(1-\epsilon)}{\epsilon^2 d_p}\rho_g u^2$$

$$\epsilon\rho_g C_{v,g}\frac{\partial T_g}{\partial t} + \rho_g C_{p,g}\frac{\partial(uT_g)}{\partial x} =$$

$$\epsilon\lambda_L\frac{\partial^2 T_g}{\partial x^2} - (1-\epsilon)\rho_p C_s\frac{\partial T_s}{\partial t} + (1-\epsilon)\rho_p\sum_j(-\nabla H_j)\frac{\partial q_j}{\partial t} - \frac{4h_w}{\epsilon d_{int}}(T_g - T_w)$$

$$\rho_p C_s\frac{\partial T_s}{\partial t} = \frac{6h_f}{d_p}(T_g - T_s) + \rho_p(-\nabla H_i)\frac{\partial q_j}{\partial_t}$$

$$\rho_w C_{p,w}\frac{\partial T_w}{\partial t} = \alpha_w h_w(T_g - T_w) - \alpha_{wi}U(T_w - T_\infty)$$

Assumptions

- From experimental data, T hardly varies so can regard as constant
- For this model, u is taken as constant but in actuality relies on C
- Ideal gas law is obeyed
- Gas, adsorbent and wall of pipe are in thermal equilibrium
- The porous adsorbent is homogeneous
- The flow is laminar
- The system is adiabatic and isothermal as the pipe is insulated and so no heat is lost

Estimation of Model Parameters

For the solving method of the equation we simplified down to one dimension in order to get the following equations:

$$\epsilon \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \epsilon D \frac{\partial^2 C}{\partial x^2} - \rho \left(1 - \epsilon\right) \frac{\partial q}{\partial t} \tag{6}$$

$$\frac{\partial q}{\partial t} = K_L(q^* - q) \tag{7}$$

Parameter Values

For the modelling of the experiments we used the following values and dimensions:

PARAMETER VALUES AND DIMENSIONS	
Parameter	**Value**
q_m	10.05
K_0	$7.62e-10$
ΔH	$-21.84e3$
K_L	0.7
R	8.314
T_g	373
c_0	0.05
ρ	1140
ϵ	0.52
D_L	$1e-5$
L	0.83

Non-Dimensionalisation

- **We considered only 1 spatial dimension**
- **The velocity is taken from experiments and found to be of order** 10^{-4}
- **We non-dimensionalised our variables using** $t' = \tau t$ **,** $q' = Qq$ **,** $C' = C_0 C$ **and** $x' = Lx$
- **We know** C_0 **is the input flow: the concentration at the start of the pipe**
- **We also know** L**: the length of the pipe.**
- **But what are** Q **and** τ**?**

Non-Dimensionalisation

- **Substituting in and removing all primes, we divide through such that the advection coefficient is 1 as we know that is what is responsible for flow. So we get**

$$\frac{L\epsilon}{u\tau}\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} = \frac{\epsilon D}{Lu}\frac{\partial^2 C}{\partial x^2} - \frac{(1-\epsilon)QL}{\tau u C_0}\frac{\partial q}{\partial t}$$

$$\frac{\partial q}{\partial t} = K_L\tau(q^* - q)$$

$$Qq^* = \frac{q_m K_{eq} RTC_0 C}{[1 + (K_{eq} RTC_0 C)^n]^{1/n}}$$

Non-Dimensionalisation

- **So we let** $Q = q_m K_{eq} RTC_0$ **and** $\tau = \dfrac{1}{K_L}$
- **So we have**

$$\frac{L\epsilon K_L}{u}\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} = \frac{\epsilon D}{Lu}\frac{\partial^2 C}{\partial x^2} - \frac{(1-\epsilon) q_m K_{eq} RTLK_L}{u}\frac{\partial q}{\partial t}$$

$$\frac{\partial q}{\partial t} = (q^* - q)$$

$$q^* = \frac{C}{[1 + (K_{eq} RTC_0 C)^n]^{1/n}}$$

Order of Magnitude Estimates

- **D, the diffusion coefficient and thus the coefficient of $\frac{\partial^2 C}{\partial x^2}$ is very small. Then, at large t, owing to a rescaling in time, the $\frac{\partial C}{\partial t}$ term also becomes small. So our first equation becomes**

$$\frac{\partial C}{\partial x} = -\frac{\partial q}{\partial t}$$

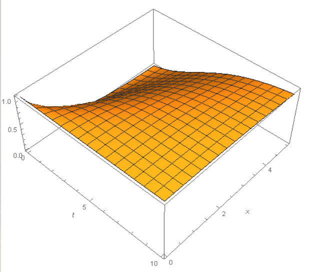
- **Next, $K_{eq}RTC_0$ is found to be very small so we have**

$$q^* \approxeq C$$

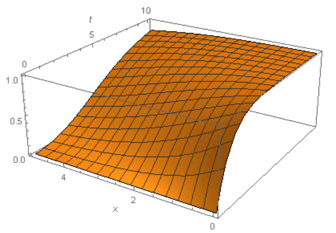
$$\frac{\partial q}{\partial t} = a_1(C - q)$$

Where a_1 is a constant.

Order of Magnitude Estimates



(a) **Concentration**



(b) **Adsorption**

Figure: Concentration and Adsorption Over Time and Space

Order of Magnitudes Estimates

At small time, when the concentration rate of change term does not fall away, a more accurate set of equations is

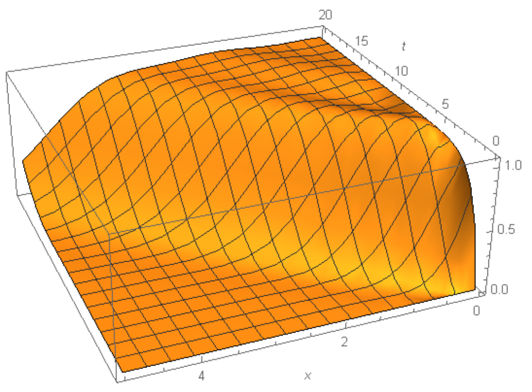
$$\beta \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} = -\frac{\partial q}{\partial t} \tag{8}$$

$$\frac{\partial q}{\partial t} = \alpha (C - q) \tag{9}$$

And, from the parameters in the table above, we found $\beta \approxeq 3$ **and** $\alpha \approxeq 1.2$ **d**

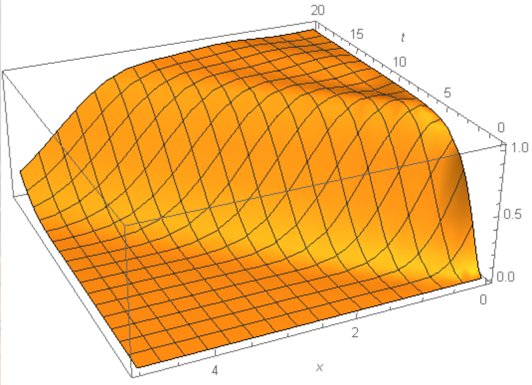
Numerical Results

- **Concentration over time and space:**



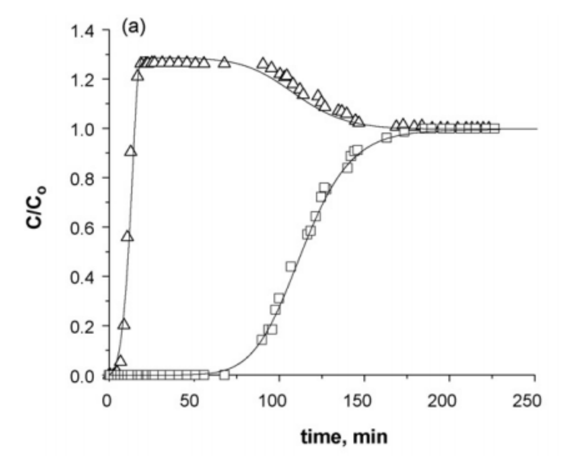
Numerical Results

- **Adsorption over time and space:**



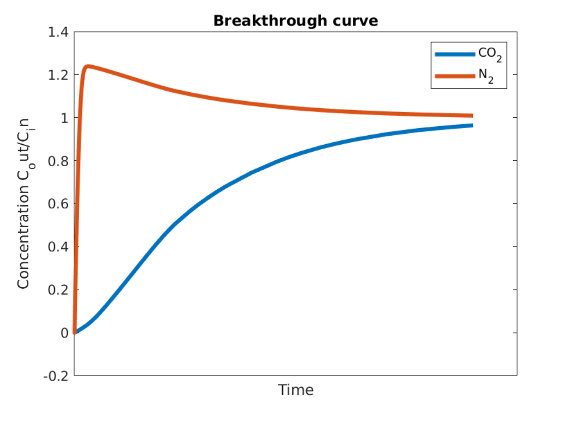
Literature Results

"Breakthrough Curve" - Squares are CO_2 and triangles are N_2:



Numerical method

Method of lines approach with a Chebyshev Spectral method in space and ODE15s in time



Conclusions

- Learned about the process of carbon capture and the various methods to achieve it
- A basic model was constructed, order of magnitude estimates were calculated and then improved upon using non-dimensionalisation
- Parameter values not clear and there were problems with units, with their varying in different experiments.
- Full numerical solution not completed in time
- We still need to consider how to store or use the captured carbon dioxide: maybe a problem for next year

Future Work

- Began looking at a solution relating the derivative of the pressure to the velocity, instead of taking u to be constant
- Now that we have a basic model, we can look at a simple way to vary the parameters to maximise carbon adsorption
- Our numerical solution was calculated much faster than the full numerical solution, and the graphs matched the literature, so we may be only missing small corrections

Thank You