

# Degree in Mathematics

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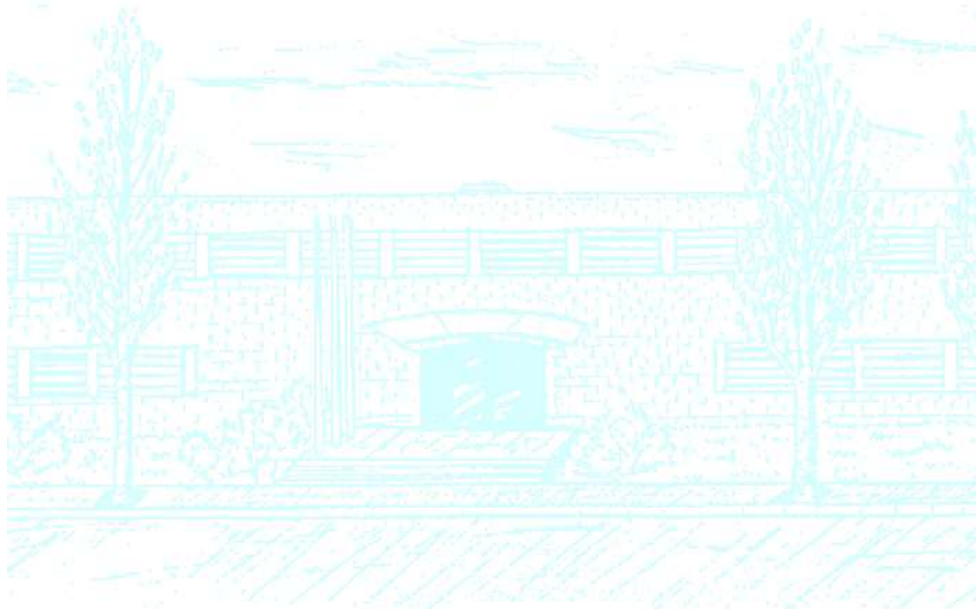
**Title: Mathematical modelling of carbon capture process by sorption**

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Universitat Politècnica de Catalunya  
Facultat de Matemàtiques i Estadística

Degree in Mathematics  
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# Mathematical modelling of carbon capture process by sorption

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Thanks to my family for helping me make progress in this work.



## **Abstract**

Concern for carbon dioxide emissions have been growing considerably during the last years and this has motivated research in topics like carbon capture. Carbon capture consists in capturing the carbon dioxide that is produced in fossil fuel plants before releasing it to the atmosphere to reduce the greenhouse effect. In this work a mathematical model for column sorption that can be applied to carbon removal by adsorption is described. After neglecting some terms of the governing equations an analytical solution for the model is shown. The breakthrough curve from the analytical solution is compared with experimental data. Finally, the existence of an analytical solution allows an analysis of the effect of the parameters to be done. With it, it is discussed which possible modifications of the parameters could be used to make the carbon dioxide removal more efficient.

## **Keywords**

carbon capture, adsorption, column sorption, mathematical model, contaminant removal

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# 1. Introduction

During the last decades carbon dioxide emissions have been increasing and the growing concern about the climate crisis has motivated the research in topics that aim to solve that. These include not only upgrades of the currently used methods that generate less carbon dioxide but also processes that actively remove CO<sub>2</sub> like carbon capture. Carbon capture consists of technologies that aim to reduce carbon emissions by capturing the CO<sub>2</sub> generated by fossil fuel plants before releasing it to the atmosphere. The stored carbon dioxide can be later used in multiple ways but it is mostly injected in deep subsurface geological formations in which the CO<sub>2</sub> is prevented from leaving.

There are three different ways in which carbon capture can be done; in each of them carbon dioxide is extracted in a different stage of energy generation. We will focus in postcombustion, where the product gas of the combustion of a fuel is treated in a way that CO<sub>2</sub> is extracted. Multiple ways of removing the CO<sub>2</sub> from the flue gas exist, such as absorption, adsorption and membrane gas separation. The most commonly used method nowadays is chemical absorption. The drawback of this method is that a lot of energy is required for the regeneration of the absorbent. For this reason a lot of alternatives have been recently explored.

The process described in this work is known as column sorption and is the most popular configuration in sorption processes. It can be used to remove carbon dioxide from a fluid but it is a general process that can be used to remove a specific component (sorbate) from a mixture by being attached to another substance (sorbent). This configuration is often used to remove organic contaminants from water.

In column sorption the removal of the pollutant is done by making the polluted fluid flow through a column filled with a porous material. This material is capable of capturing the pollutant as it passes through the column in two different ways: by absorption, the pollutant gets into the holes of the porous material; and by adsorption, the pollutant is adhered to the surface. Even though the mathematical part could describe both adsorption or absorption, in the capture process that is being discussed in this work the removal of the contaminant is done only by adsorption.

## 2. Objectives

The objective of this work is to provide a way to predict the behaviour of the process by describing how the concentration in the column changes and to determine how the parameters should be modified in order to optimise the removal of the contaminant.

To do this a mathematical model will be first developed and non-dimensionalised, then an analytical approximate solution will be shown. With an exact expression for the concentration of CO<sub>2</sub> at the outlet of the column a comparison with experimental data will be done. The data that will be used is from [3] where a mixture gas containing CO<sub>2</sub> and N<sub>2</sub> that simulates a flue gas of a power plant was used. The exact expression will also allow us to do an analysis on the effect of each parameter and state how they should be modified in order to optimise the process of carbon capture.

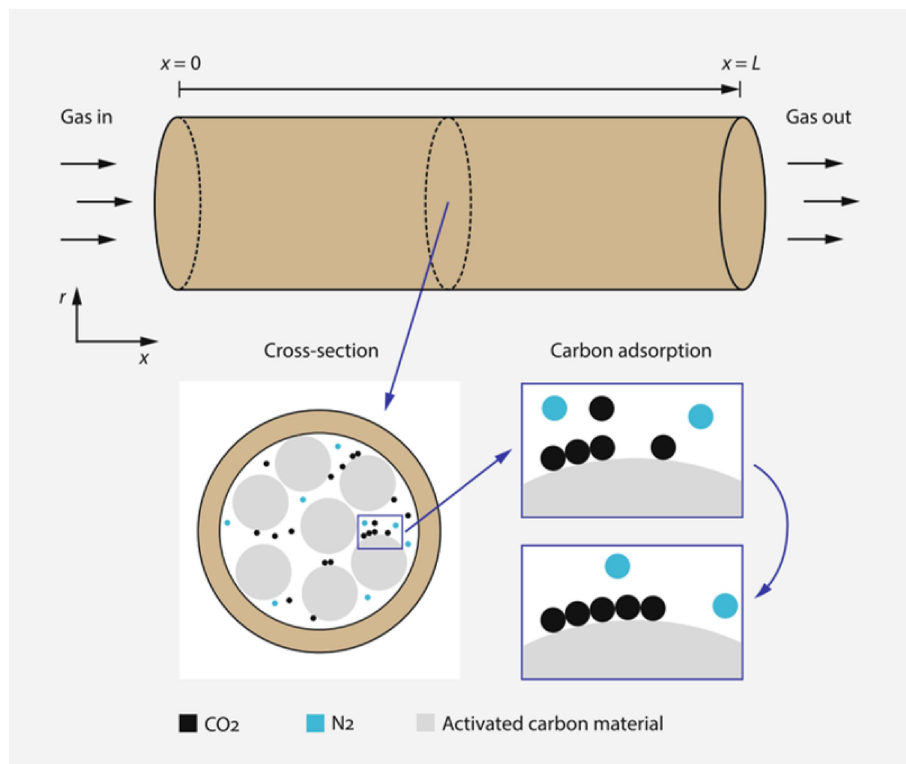


Figure 1: Configuration of the process, image from [2]

### 3. Mathematical model

The mathematical model described in this section is a simplification of the model from [1] since here pressure will not be taken into account.

Let's consider a cylinder that contains the adsorbent material with both ends open with a flux through it. The fluid that comes into this column will have some concentration of the pollutant we want to remove. We will assume that the concentration of the pollutant does not depend on the radial component and the flow through the column is a plug flow, that means that the velocity field inside the column is parallel to the column and does not depend on the radial component. With these assumptions the problem will be reduced to a one-dimensional problem in space.

We will consider the  $x$ -axis the only axis of the problem, the one that is parallel to the column. All the variables will be assumed to depend only on  $x$  and time  $t$ , that is, they are defined as averages over sections of the column.

Conservation of mass for the pollutant gives the equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = S \quad (1)$$

where  $\rho$  is the density of the fluid,  $j$  is the flux and  $S$  is the sink of mass, which represents the amount of pollutant that is removed from the fluid. Since the flow inside is affected by diffusion and advection, the flux  $j$  is

$$j = -D\nabla\rho + \rho\mathbf{u} \quad (2)$$

where  $D$  is the diffusion coefficient (in the  $x$  direction) and  $\mathbf{u}$  is the velocity field. Since we are assuming plug flow,  $\mathbf{u}(x, t) = (u(x, t), 0, 0)$ .

If  $\bar{q}$  denotes the amount of moles of pollutant adsorbed by the solid per kilogram of this solid then the source term

$$S = -(1 - \varepsilon)\rho_q M_1 \frac{\partial \bar{q}}{\partial t}. \quad (3)$$

Here  $\varepsilon$  is the bed void fraction, the fraction of volume of the cylinder that is not occupied by the adsorbent solid.  $\rho_q$  denotes the density of the solid when it has adsorbed pollutant and  $M_1$  is simply the molar mass of the pollutant. The bar in  $\bar{q}$  indicates that it is taken as a cross-sectional average in order to avoid the radial dependence of  $q$ . After using the forms of the field  $\mathbf{u}$  and the source  $S$  and writing the density as  $\rho = M_1 c_1$  where  $c_1$  is the concentration in moles per volume, the equation (1) is

$$\frac{\partial c_1}{\partial t} + \frac{\partial}{\partial x}(u c_1) = D \frac{\partial^2 c_1}{\partial x^2} - (1 - \varepsilon)\rho_q \frac{\partial \bar{q}}{\partial t}. \quad (4)$$

For the mass transfer we will use the linear driving force model; we will assume that the rate of mass transfer is proportional to the free sites in the solid,

$$\frac{\partial \bar{q}}{\partial t} = k_q(\bar{q}^* - \bar{q}) \quad (5)$$

where  $k_q$  is the rate constant and the  $\bar{q}^*$  is the maximum value of  $\bar{q}$ , the saturation value. This equation only applies where mass transfer can occur, where there is pollutant in the fluid to be adsorbed ( $c_1 > 0$ ).

In the region where  $c_1 = 0$  the amount of adsorbed mass remains constant. Apart from this,  $\bar{q}^*$  usually depends on time and space so the equation cannot be directly integrated. Even though there are simpler models that assume that the equilibrium between fluid and adsorbed phase is always maintained and more complex models that take into account the internal structure of the solid particles, the linear driving force model or modifications of it are the most commonly used mass transfer models for adsorption processes.

At the inlet,  $x = 0$ , we have to apply a boundary condition for the continuity of mass flux. We impose that the flux on both sides of the inlet is the same.

$$u(0^-, t)c_{10} = \left( uc_1 - D \frac{\partial c_1}{\partial x} \right) \Big|_{x=0^+} \quad (6)$$

where  $c_{10}$  is the concentration of pollutant of the fluid that enters and the  $0^-$  and  $0^+$  indicate limits from left and right sides of the inlet. At the end of the column we impose that, since the fluid moves to a region where there is no mass sink, the concentration  $c_1$  remains the same outside the exit.

$$\frac{\partial c_1}{\partial x} \Big|_{x=L^-} = 0 \quad (7)$$

For the times before the pollutant has reached the end of the column we need to impose another condition at the front of the concentration,

$$\frac{\partial c_1}{\partial x}(s(t), t) = c_1(s(t), t) = 0, \quad (8)$$

$$\bar{q}(s(t), t) = 0. \quad (9)$$

Here  $s(t)$  is the front of the concentration, that is the furthest point in the column where  $c_1 > 0$ , or the closest point to the entrance where  $c_1 = 0$ . Trivially, at the beginning of the process  $s(t)$  will be 0 and it will increase gradually. For the initial conditions we impose that the column is clean before the flux of the polluted fluid.

$$\bar{q}(x, 0) = 0, \quad c_1(x, 0) = 0, \quad \forall t \geq 0. \quad (10)$$

As it has been commented before, some of the parameters can actually depend on the temperature and the pressure. We will assume that they are both constant but since adsorption is an exothermic process an energy balance could be taken into account in order to get more precise results.

## 4. Non-dimensionalisation

With the non-dimensional analysis we can simplify the problem by removing negligible terms. For this we will need to use actual parameters of the experiment. These values are the ones in table 1 and are corresponding to the experiment done in [3].

We can define new non-dimensional variables as

$$\hat{c}_1 = \frac{c_1}{c_{10}}, \quad \hat{q} = \frac{\bar{q}}{\bar{q}_0^*}, \quad \hat{u} = \frac{u}{u_0}, \quad \hat{x} = \frac{x}{\mathcal{L}}, \quad \hat{t} = \frac{t}{\Delta t} \quad (11)$$

where  $c_{10}$  is the concentration of pollutant in the fluid that comes into the column,  $\bar{q}_0^*$  is the value of  $\bar{q}^*$  at time 0 and the other parameters are yet to determine. With them we can get new equations on these variables with non-dimensional factors that indicate the relative importance of the terms.

The new equations are

$$\delta_1 \frac{\partial \hat{c}_1}{\partial \hat{t}} + \delta_2 \frac{\partial}{\partial \hat{x}} (\hat{u} \hat{c}_1) = \delta_3 \frac{\partial^2 \hat{c}_1}{\partial \hat{x}^2} - \frac{\partial \hat{q}}{\partial \hat{t}} \quad (12)$$

$$\frac{\partial \hat{q}}{\partial \hat{t}} = k_q \Delta t (\hat{q}^* - \hat{q}) \quad (13)$$

where

$$\delta_1 = \frac{c_{10}}{(1 - \varepsilon) \rho_q \bar{q}_0^*}, \quad \delta_2 = \frac{u_0 c_{10} \Delta t}{\mathcal{L} (1 - \varepsilon) \rho_q \bar{q}_0^*}, \quad \delta_3 = \frac{D c_{10} \Delta t}{\mathcal{L}^2 (1 - \varepsilon) \rho_q \bar{q}_0^*}. \quad (14)$$

To balance the second equation we have to make  $k_q \Delta t = 1$ . By defining  $\Delta t = \frac{1}{k_q}$  we will get the balanced equation.

$$\frac{\partial \hat{q}}{\partial \hat{t}} = \hat{q}^* - \hat{q} \quad (15)$$

The parameter  $\bar{q}^*$  can vary with the temperature, the pressure and the concentration  $c_1$ . However we will assume that it is constant as a first approach. This means that  $\hat{q}^* = 1$ .

In the first equation we can balance the advection and mass loss terms, that is making  $\delta_2 = 1$  by defining the parameter  $\mathcal{L}$  introduced in the new variables as

$$\mathcal{L} = \frac{u_0 c_{10}}{(1 - \varepsilon) \rho_q \bar{q}_0^* k_q}. \quad (16)$$

This leads to a new equation with only  $\delta_1$  and  $\delta_3$  as coefficients of the terms different from 1. The new system of equations is

$$\delta_1 \frac{\partial \hat{c}_1}{\partial \hat{t}} + \frac{\partial}{\partial \hat{x}} (\hat{u} \hat{c}_1) = \delta_3 \frac{\partial^2 \hat{c}_1}{\partial \hat{x}^2} - \frac{\partial \hat{q}}{\partial \hat{t}} \quad (17)$$

$$\frac{\partial \hat{q}}{\partial \hat{t}} = 1 - \hat{q} \quad (18)$$

Using the values from the table below  $\delta_1$  and  $\delta_3$  are

$$\delta_1 = 0.0269, \quad \delta_3 = 0.0363. \quad (19)$$

The fact that they are small means that the respective terms in the equation do not play an important role so they can be neglected. However we will only remove the diffusive term because it is enough to provide the travelling wave solution. The resulting system of equations is

$$\frac{\partial}{\partial \hat{x}}(\hat{u}\hat{c}_1) = -\frac{\partial \hat{q}}{\partial \hat{t}} \quad (20)$$

$$\frac{\partial \hat{q}}{\partial \hat{t}} = 1 - \hat{q}. \quad (21)$$

The boundary conditions become, with the non-dimensionalised variables,

$$\hat{u}(0^-, \hat{t}) = \left( \hat{c}_1 - \delta_3 \frac{\partial \hat{c}_1}{\partial \hat{x}} \right) \Big|_{\hat{x}=0^+}, \quad (22)$$

$$\frac{\partial \hat{c}_1}{\partial \hat{x}}(\hat{s}(\hat{t}), \hat{t}) = \hat{c}_1(\hat{s}(\hat{t}), \hat{t}) = 0, \quad (23)$$

$$\frac{\partial \hat{c}_1}{\partial \hat{x}} \Big|_{\hat{x}=\hat{L}=L^-/L} = 0. \quad (24)$$

The term with the  $\delta_3$  can be neglected since it is the same order as the diffusive term, that has been neglected.

Parameter	Symbol	Value	Dimension
Initial concentration	$c_{10}$	6.03	mol/m <sup>3</sup>
Adsorption saturation	$\bar{q}^*$	1.57	mol/kg
Bed void fraction	$\varepsilon$	0.56	
Density of adsorbed CO <sub>2</sub>	$\rho_q$	325	kg/m <sup>3</sup>
Diffusion coefficient	$D$	$2.57 \cdot 10^{-5}$	m <sup>2</sup> /s
Bed length	$L$	0.2	m
Interstitial velocity	$u$	0.019	m/s
Adsorption rate constant	$k_q$	0.0137	s <sup>-1</sup>

Table 1: Table with the values of the parameters taken from [1].

## 5. Solution for constant velocity

Assuming that the velocity field is constant in space and time, a valid hypothesis when small amount of contaminant is being removed,  $\hat{u} = 1$ , the system describing the problem is the following,

$$\delta_1 \frac{\partial \hat{c}_1}{\partial \hat{t}} + \frac{\partial \hat{c}_1}{\partial \hat{x}} = -\frac{\partial \hat{q}}{\partial \hat{t}}, \quad (25)$$

$$\frac{\partial \hat{q}}{\partial \hat{t}} = 1 - \hat{q}. \quad (26)$$

We will look for a solution in the form of a travelling wave, which means that the solution, in this case the variables  $\hat{c}_1$  and  $\hat{q}$ , can be expressed as a function of one variable  $\hat{\eta} = \hat{\eta}(\hat{x}, \hat{t}) = \hat{x} - \hat{s}(\hat{t})$  where  $\hat{s}(\hat{t})$  is the front of  $\hat{c}_1$ .

$$\hat{c}_1(\hat{x}, \hat{t}) = f(\hat{\eta}) = f(\hat{x} - \hat{s}(\hat{t})), \quad (27)$$

$$\hat{q}(\hat{x}, \hat{t}) = g(\hat{\eta}) = g(\hat{x} - \hat{s}(\hat{t})). \quad (28)$$

The fact that the solution is a travelling wave means that the distributions of  $\hat{c}_1$  and  $\hat{q}$  in space conserve the shape and this shape travels at the same speed as the front of the concentration  $\hat{s}(\hat{t})$ .

By assuming that the solution has this form the equations can be rewritten as

$$-\delta_1 \frac{d\hat{s}}{d\hat{t}} \frac{df}{d\hat{\eta}} + \frac{df}{d\hat{\eta}} = \frac{d\hat{s}}{d\hat{t}} \frac{dg}{d\hat{\eta}}, \quad (29)$$

$$-\frac{d\hat{s}}{d\hat{t}} \frac{dg}{d\hat{\eta}} = 1 - g. \quad (30)$$

Note that since  $\hat{s}(\hat{t})$  is the front of the pollutant concentration, the boundary condition at this point ( $\hat{x} = \hat{s}(\hat{t})$ ) translates to an initial condition for the  $f$  and  $g$  functions at  $\hat{\eta} = 0$  which is

$$f(0) = g(0) = 0. \quad (31)$$

If the pollutant front is moving at constant speed then  $\frac{d\hat{s}}{d\hat{t}} = v$  constant and the the first equation, with the boundary condition  $f(0) = g(0) = 0$ , implies that  $(1 - \delta_1 v)f = v g$ .

The second equation can be integrated exactly and the solution after applying the initial condition is

$$g(\hat{\eta}) = 1 - e^{\hat{\eta}/v}, \quad (32)$$

so

$$f(\hat{\eta}) = \frac{v}{1 - \delta_1 v} (1 - e^{\hat{\eta}/v}). \quad (33)$$

Assuming  $\hat{s}(\hat{t})$  is far enough from the entrance,  $\hat{x} = 0$ , the entrance corresponds to  $\hat{\eta} = 0 - \hat{s}(\hat{t})$  which is negative and large which means that  $e^{\hat{\eta}/v}$  is small so we can approximate  $\hat{u}\hat{c}_1 = \hat{c}_1$  at this point as

$$\hat{c}_1(0, \hat{t}) = f(\hat{\eta}) = \frac{v}{1 - \delta_1 v} (1 - e^{\hat{\eta}/v}) \approx \frac{v}{1 - \delta_1 v}. \quad (34)$$

Because of how the non-dimensional variables have been defined,  $\hat{c}_1(0, \hat{t}) = 1$  and that implies that  $v = \frac{1}{1 + \delta_1}$ . This allows us to write  $f$  with a simpler expression

$$f(\hat{\eta}) = 1 - e^{\hat{\eta}/v}. \quad (35)$$

Note that  $f = g$  so we expect the concentration of the contaminant  $\hat{c}_1$  and the adsorbed mass  $\hat{q}$  to behave in a very similar way.

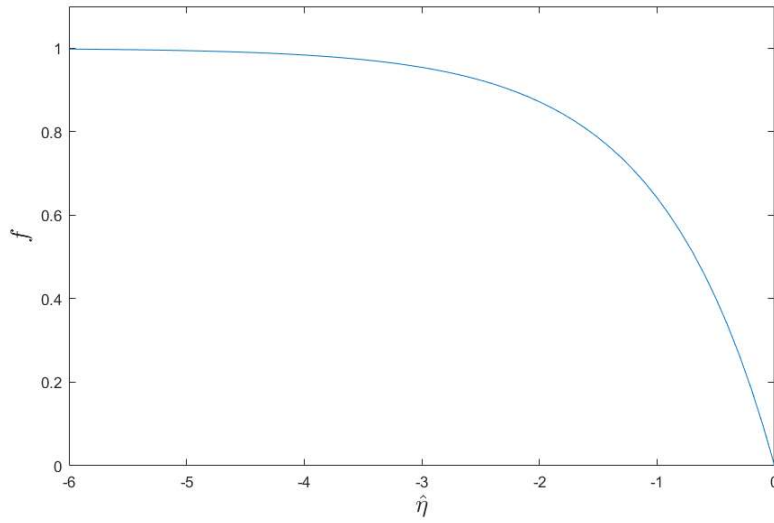


Figure 2: Shape of the profile of concentration  $\hat{c}_1$  and  $\hat{q}$ .

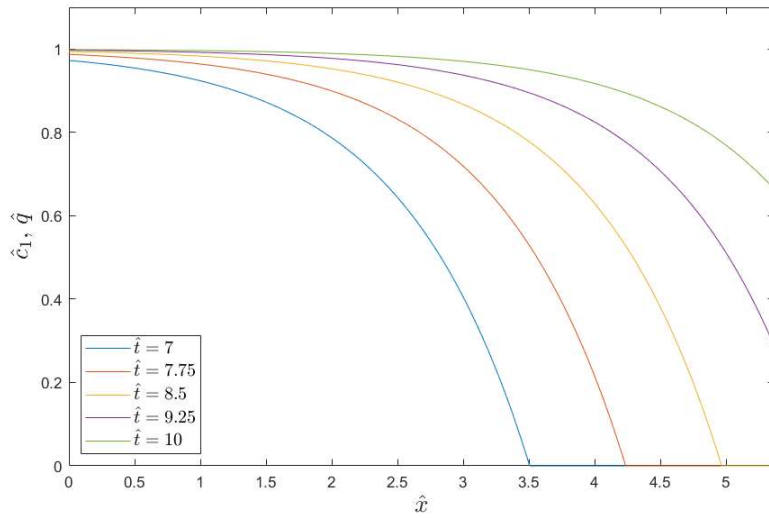


Figure 3: Travelling wave solution for  $\hat{c}_1$  and  $\hat{q}$  at some times.

The expression for  $\hat{c}_1$  (and  $\hat{q}$ ) is not completely explicit because in order to write  $\hat{s}(\hat{t})$  we need to know the initial value  $\hat{s}_0$  apart from the constant velocity that we know. Since the travelling wave solution is not valid when  $\hat{s}(\hat{t})$  is close to 0, and thus not valid at initial times we cannot set  $\hat{s}_0 = 0$ . To determine the value of  $\hat{s}_0$  we need to make use of the experimental data. One way to do this is by measuring the first time  $t_b$  that the pollutant reaches the outlet. Then we can set the dimensional front  $s_0 = L - vt_b$  so  $s(t_b) = L$ . Another way to do this is by using the time  $t_{1/2}$  at which the concentration at the outlet first reaches one half of the initial concentration. Imposing this to the equation (35) leads to  $\hat{s}_0 = \hat{L} - \hat{v}\hat{t}_{1/2} + \hat{v} \log 2$ .



This solution is only valid when the front of the  $\hat{c}_1$  is not close to the entrance, so it must have passed some time since the start of the process. This is not an issue because the main interest is in the breakthrough curve, the curve that represents evolution of the concentration at the exit of the column, which becomes non-zero only after the front reaches the outlet and this happens far from the beginning. Even though a solution for the start of the process is not needed, a good approximation for small times exists.



## 6. Solution for small times

When little time has passed since the start of the process, the amount of adsorbed mass  $\hat{q}$  is small. So we can rescale this variable and time

$$\hat{t} = \epsilon \hat{\tau}, \quad \hat{q} = \epsilon \hat{Q}. \quad (36)$$

The equation (26) with the rescaled variables becomes

$$\frac{\partial \hat{Q}}{\partial \hat{\tau}} = 1 - \epsilon \hat{Q} \quad (37)$$

with the condition  $Q(\hat{\tau}_s) = 0$ . The main equation (37) can be expanded as a sum of powers of  $\epsilon$ . If we neglect  $\epsilon$ , (we take only the first term of the series) the solution is

$$\hat{Q} = \hat{\tau} - \hat{\tau}_s. \quad (38)$$

The same can be done for the concentration  $\hat{c}_1$ . The concentration does not need to be rescaled since it must be close to 1 near the entrance. The equation (17), with the diffusive term already neglected, becomes

$$\frac{\delta_1}{\epsilon} \frac{\partial \hat{c}_1}{\partial \hat{\tau}} + \frac{\partial}{\partial \hat{x}} (\hat{u} \hat{c}_1) = -\frac{\partial \hat{Q}}{\partial \hat{\tau}}. \quad (39)$$

By considering the approximation for  $\hat{Q}$  (or neglecting  $\epsilon$ ), the derivative  $\frac{\partial \hat{Q}}{\partial \hat{\tau}}$  is 1 and is constant. In this case if we take  $\epsilon$  big enough we can make the coefficient  $\frac{\delta_1}{\epsilon}$  negligible. For example we can take  $\epsilon = \sqrt{\delta_1}$ . With this the general solution for the equation is

$$\hat{c}_1 = A - \hat{x}. \quad (40)$$

To determine the values of  $A$  we have to make use of the boundary conditions of the problem. Using (22), that is now simply

$$1 = \hat{c}_1 \Big|_{\hat{x}=0}, \quad (41)$$

so

$$A = 1. \quad (42)$$

With this exact expression for  $\hat{c}_1$  we can see that during this initial phase the concentration front  $\hat{s}(\hat{t})$  is 1 and it is constant.

In addition to being able to complete the travelling wave solution, this small time solution is usually useful to set an initial value for a numerical solution.

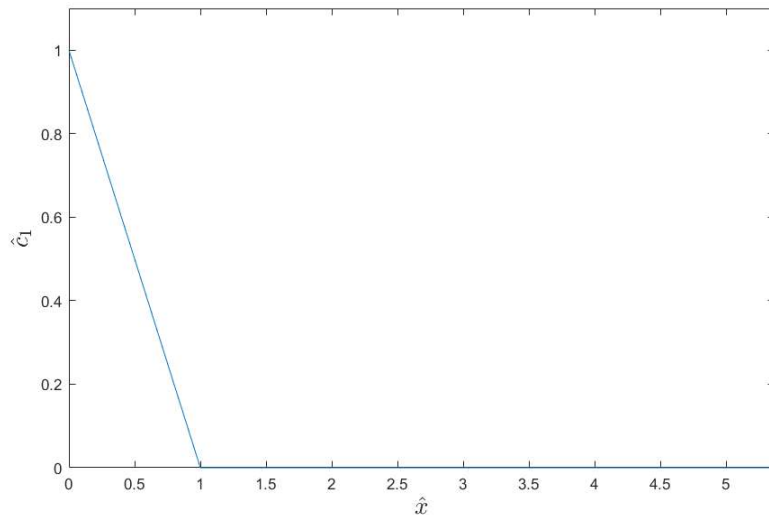


Figure 4: Concentration in the fluid at  $\hat{t} = \sqrt{\delta_1} = 1.6389$  and during the initial phase.

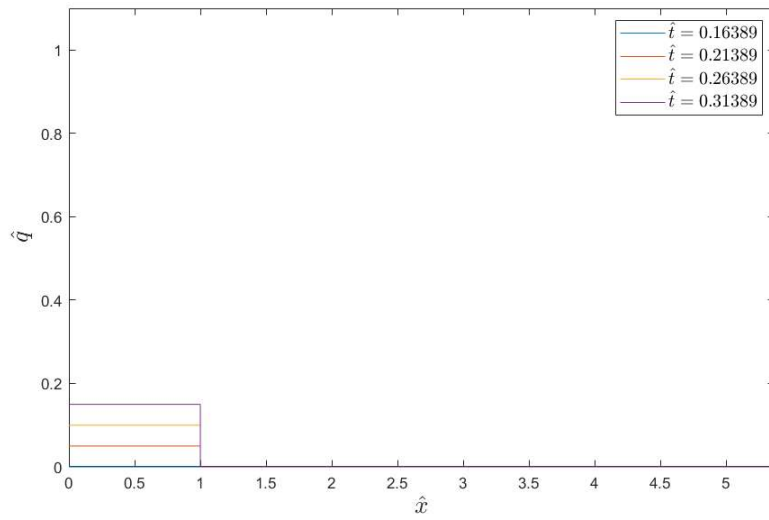


Figure 5: Adsorbed mass  $\hat{q}$  during the initial phase.

## 7. Comparison with experimental data

Given the parameters we can compare the analytical solution that we have with data measured in a real experiment to see if the approximation is good. A typical way to compare two different solutions is by comparing the behaviour of the concentration at the exit of the column, known as the breakthrough curve.

In this case the data used in the comparison is from the experiment from [3]. In this experiment the gas that is fed to the column is a mixture of N<sub>2</sub> and CO<sub>2</sub>, that is a typical flue gas of postcombustion.

The analytical expression for the concentration of CO<sub>2</sub> at the outlet of the column in dimensional form is

$$c_1(L, t) = c_{10} \left( 1 - \exp \left( k_q \frac{L - s_0 - vt}{v} \right) \right), \quad (43)$$

where

$$v = \frac{1}{\mathcal{L}k_q(1 + \delta_1)}. \quad (44)$$

Not all parameters that appear in the expression are known. Some of them have been taken from [1] where the parameter  $k_q$  was calculated in order to fit optimally experimental data. The model used there is not the same that has been presented in this work. For this reason, in this section we will treat the rate constant as another unknown parameter.

Apart from that, an initial value for the front of the concentration of the pollutant must be set. This parameter should be obtained from the experimental data. If we define  $t_b$  as the first time the pollutant is detected in the outlet then we set  $s_0 = L - vt_b$ , so the front  $s(t)$  reaches the outlet at time  $t_b$ .

With this approximation for  $s_0$  we can find the optimal  $k_q$  value. As it can be seen in figure 6 the general shape of both curves are similar but the analytical solution fails to predict the time of first breakthrough. The rise of the concentration at time  $t_b$  is smoother than the one of the analytical solution.

Since the measurements of the concentration are done in a discrete way the value for  $s_0$  that we obtain by using the experimental first breakthrough time is not optimal and not precise. An optimal value of  $s_0$  can be found such that the analytical solution fits the experimental data.

However, by using a better value for  $k_q$  and  $s_0$  none of the main issues of the analytical breakthrough curve seem to disappear. The experimental curve is still too smooth and there is no way to change that in the analytical solution with our parameters without changing the model.

One of the factors that could affect the results is having neglected velocity variation. Removing part of the mass of the flowing gas has an effect on its velocity that has been considered negligible. At the front of  $s(t)$  the loss of mass due to adsorption is balanced with a decrease of the velocity.

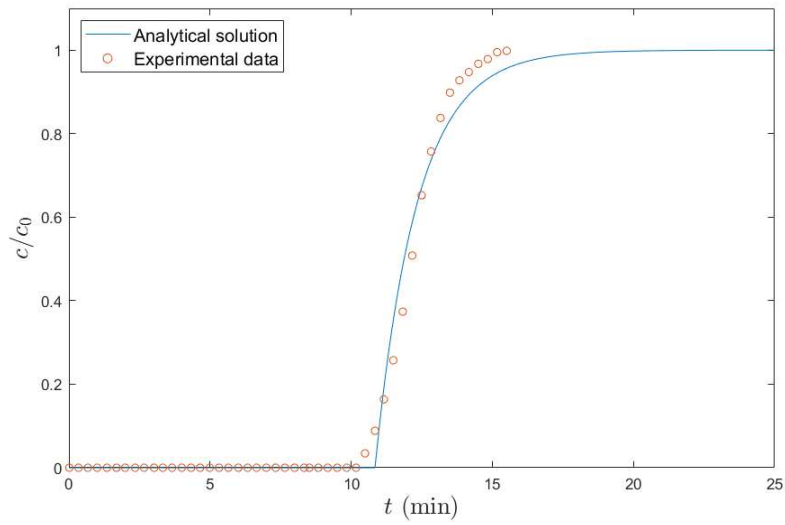


Figure 6: Comparison between the analytical solution and the experimental data with  $k_q$  such that analytical solution fits the experimental data and  $s_0 = L - vt_b$ .

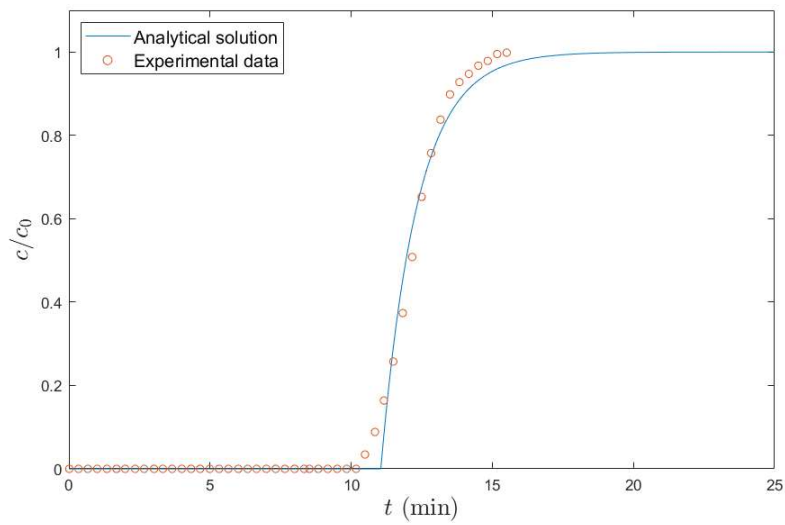


Figure 7: Comparison between the analytical solution and the experimental data with  $k_q$  and  $s_0$  such that analytical solution fits the experimental data.

## 8. Possible improvements

The goal of this section is to determine how the parameters should be modified in order to make the removal of a contaminant more efficient. For this we will make use of the analytical solution. With its expression it can be seen how each parameter affects the solution. The concentration of pollutant at the outlet is the expression that will be of interest.

$$c_1(L, t) = c_{10} \left( 1 - \exp \left( k_q \frac{L - s_0 - vt}{v} \right) \right), \quad (45)$$

$$v = \frac{(1 - \varepsilon)\rho_q \bar{q}_0^*}{(1 + \delta_1)u_0 c_{10}}. \quad (46)$$

What can be improved in the described process is the speed at which column is filled with the adsorbed pollutant. It is clear that we can accelerate the process by increasing the rate constant  $k_q$ , which will make the contaminant be adsorbed faster. But in order to see how each parameter affects this speed we will define the time at which we can consider that the process has ended. This time will be when the concentration at the end of the column is 90% of the concentration of the fluid entering the column. In order to speed up the process we will try to make this time as small as possible. To see the dependence on the parameters we will make use of the analytical solution. Since the initial time solution occupies only a small part of the total process its effect will be neglected. In addition, the small time solution makes the results too complicated and confusing.

If the condition of the concentration at the end of the column is imposed on the travelling wave solution we obtain the following dimensional time.

$$t = \frac{L - s_0}{v} - \frac{1}{k_q} \log 0.1 = \frac{L - s_0}{v} + \frac{1}{k_q} \log 10 \quad (47)$$

So in order to make the time lower we have to increase  $k_q$  or  $v$ .  $v$  is the (dimensional) constant speed of concentration front.

$$v = \frac{\mathcal{L}}{\Delta t} \hat{v} = \frac{\mathcal{L}}{\Delta t(1 + \delta_1)} = \frac{\cancel{k_q} u_0 c_{10}}{(1 - \varepsilon)\rho_q \bar{q}_0^* \cancel{k_q} (1 + \delta_1)} = u_0 \frac{\delta_1}{1 + \delta_1} \quad (48)$$

Since  $\frac{\delta_1}{1 + \delta_1}$  is always increasing as a function of  $\delta_1$  we need that the parameters  $\delta_1$  and  $u_0$  are as large as possible. Since

$$\delta_1 = \frac{c_{10}}{(1 - \varepsilon)\rho_q \bar{q}_0^*}, \quad (49)$$

$c_{10}$  and  $\varepsilon$  should be large and  $\rho_q$  and  $\bar{q}_0^*$  should be small. Note that even though making  $\bar{q}_0^*$  makes the process shorter having a small value of  $\bar{q}_0^*$  is not what we want. The process is shorter because the column has less space to fill with contaminant. This parameter indicates the maximum capacity of the column so we want to keep it large. In fact the total amount of adsorbed pollutant at some time is

$$\int_0^L \bar{q} dx. \quad (50)$$

The maximum value of this is  $L\bar{q}_0^*$  since  $\bar{q}_0^*$  is the maximum value of  $\bar{q}$ . However this limit can't be reached in finite time. In the analytical solution it can be seen that  $\hat{q} = 1$  only when  $\hat{x} - \hat{s}(\hat{t}) = \hat{\eta} = -\infty$ , which means that the front  $\hat{s}(\hat{t})$  has to be far ahead from  $\hat{x}$  and that happens when a lot of time has passed. So, trivially, in order to increase the global capacity the length of the column  $L$  and the amount of adsorbed mass per mass of solid at equilibrium  $\bar{q}_0^*$  have to be increased.



## 9. Conclusions

In this work one possible way using carbon capture in a power plant has been described and mathematically modelled. With this model it has been shown that an analytical solution can be found when some terms of the advection-diffusion equation are neglected.

It has been seen that there is agreement between the proposed analytical solution and real experiment. However, even with  $k_q$  and  $s_0$  chosen to fit the data there are considerable differences around first breakthrough between both breakthrough curves. A possible cause of this discrepancy is the fact that the velocity field of the fluid has been considered uniform both in time and space. This assumption is valid only when the amount of mass adsorbed is small.

Because of the agreement with the experimental data the analytical expression for  $c_1$  can be used to discuss the dependence on the parameters. For this reason conclusions about the choice of the parameters have been shown. The adsorption process is more efficient, is either faster or has more capacity when one of the following changes to the parameters are done:

- The rate constant  $k_q$  is increased
- The velocity of the fluid  $u_0$  increases.
- The bed void fraction  $\varepsilon$  increases.
- The initial concentration  $c_{10}$  increases.
- The density of the adsorbed mass  $\rho_q$  increases.
- The length of the bed  $L$  increases.
- The amount of adsorbed mass per mass of solid at equilibrium  $\bar{q}_0^*$  increases.

The choice of some of parameters is in reality something that cannot be chosen freely because only a few materials can be used as adsorbents. Even though these indications can help to choose the optimal material among the diversity of existing ones. It can also be used to set the optimal conditions in which the carbon capture can take place since properties of the materials, such as  $\bar{q}_0^*$ , may depend on these conditions.

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