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Project 1:
One-dimensional diffusion model for CO_2 absorption in the ocean

Tor Nordam

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1 Introduction

The ocean has the capacity to absorb CO_2 from the atmosphere. This has important consequences for the climate, and hence it is of great interest for climate modellers to be able to predict the amount of CO_2 that will be absorbed from the atmosphere to the ocean. A good understanding of this process will allow us to make better predictions of how the climate will change in the future, under different scenarios for release of CO_2 into the atmosphere.

In this project, we will look at a simplified, one-dimensional model of the ocean, and study how CO_2 is absorbed at the surface, dissolved in the water, and transported down to greater depths by diffusion.

1.1 Model background

We will use what is called a "water column model", which means that we study a column of water reaching from the surface to the sea floor. We assume that everything is constant in the horizontal directions, which means that we can treat our system as one-dimensional, looking only at how conditions change with depth (and time). Describing the ocean as one-dimensional is of course a very large simplification, but it is nevertheless possible to apply a one-dimensional model to at least parts of the ocean, and qualitatively study some of the relevant processes.

In Fig. 1, the system we will study is illustrated. CO_2 may leave the atmosphere and enter the ocean surface, where it is stored as so-called *dissolved inorganic carbon*. We wish to calculate how the concentration of dissolved inorganic carbon $C(z,t)$ changes with depth and time, and how much CO_2 enters the ocean. The processes that govern this are the mass transfer across the air–sea interface, and diffusion in the water column. Mass transfer is the process by which CO_2 is absorbed from the atmosphere into the ocean (or released from the ocean to the atmosphere if the concentration in the surface water exceeds the equilibrium concentration). Diffusion is a transport process that tends to move material from regions of high concentration to regions of lower concentration.

As a side note, we point out that what we here call diffusion is in reality a combination of molecular diffusion, caused by the random motion of molecules, and turbulent mixing, which is caused by random eddying motion in the water. The combination of these effects leads to far more efficient mixing than just the molecular diffusion alone. You can observe this for example if you add milk to your tea. If you just pour in a splash of milk, thin filaments of milk may persist for quite some time, but if you stir the tea with a spoon it will mix to a homogeneous distribution almost instantly. For further details on turbulent mixing in the context of the ocean, see *e.g.*, Thorpe (2005).

2 Theory

This section presents the diffusion equation, and some other equations and parameters that will be used in our model. The focus here is on the theory, and a detailed description of how to implement this model numerically is found in the Appendix.

2.1 The diffusion equation

In this project, we will be solving the diffusion equation:

$$\frac{\partial C(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial C(z,t)}{\partial z}\right). \tag{1}$$

This is a partial differential equation (PDE), which describes how the concentration $C(z,t)$ of some species changes in space and time. Here, $K(z)$ represents the diffusivity, or the intensity of the mixing, which changes with depth.
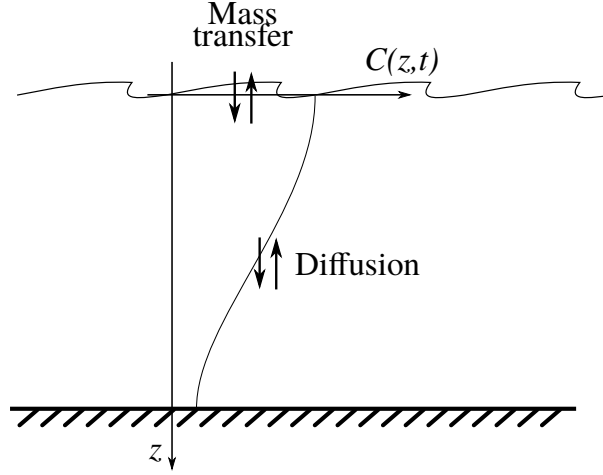
Figure 1: The figure illustrates the two processes we will consider. CO_2 enters the ocean via mass transfer across the air–sea interface. In the ocean, CO_2 is stored as dissolved inorganic carbon, the concentration of which will vary over time due to diffusion in the water column. Note that z is 0 at the surface, and positive downwards.

2.2 Boundary conditions

In addition to the diffusion equation itself, which describes what happens in the water column, we need boundary conditions to describe what happens at the boundaries of our model domain, *i.e.*, at the sea floor and at the surface.

2.2.1 Sea floor boundary

At the sea floor, at depth $z = L$, we will use a no-flux boundary condition, which simply means there is no diffusive flux through the bottom boundary. The flux due to diffusion, j_D, in a system governed by Eq. (1), is given by Fick's law[1]:

$$j_D = -K(z)\frac{\partial C(z,t)}{\partial z}. \tag{2}$$

2.2.2 Sea surface boundary, dissolved inorganic carbon, and mass transfer

At the sea surface, there is a flux j_{mt} (units $\mathrm{mol\,m^{-2}\,s^{-1}}$) of CO_2 that enters (or leaves) the ocean due to mass transfer. In the ocean, the CO_2 is stored as *dissolved inorganic carbon* (DIC). The flux is proportional to the difference between the current concentration of DIC, and the equilibrium concentration C_{eq}:

$$j_{mt} = -k_w\left(C_0 - C_{eq}\right), \tag{3}$$

where k_w is the mass transfer coefficient, C_0 is the concentration of DIC in the water just below the surface (at depth $z = 0$). Hence, the flux is positive (directed downwards, into the sea) if $C_0 < C_{eq}$, and negative (directed upwards, into the atmosphere) if $C_0 > C_{eq}$.

The equilibrium concentration C_{eq} is a function of the partial pressure p_{CO_2} of CO_2 in the atmosphere. Additionally, it depends on the solubility of CO_2, and carbonate chemistry. When CO_2 dissolves into water, an equilibrium is established where the CO_2 is partially transformed into H_2CO_3, HCO_3^-, and CO_3^{2-}, via chemical reactions with the water. These compounds are what is collectively known as dissolved inorganic carbon[2]. The exact proportions of these compounds depend on local conditions (particularly temperature and pH), but the details are a bit complicated[3]. However, when the ocean absorbs CO_2, only about 1% or less of the absorbed molecules are actually present as dissolved pure CO_2. The majority of the mass is stored in the form of H_2CO_3, HCO_3^-, and CO_3^{2-}. Hence, we must take this into account in our calculations, if we wish to estimate the amount of CO_2 the ocean can absorb.

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[1] https://en.wikipedia.org/wiki/Fick's_laws_of_diffusion
[2] https://en.wikipedia.org/wiki/Dissolved_inorganic_carbon
[3] For the interested reader, Zeebe (2012) gives a nice and readable overview of carbonate chemistry in the ocean.

For the purposes of this project, we will make the following simplification: We will assume that when CO_2 enters the ocean, it is immediately transformed into DIC, and we will simulate the changing concentration of DIC with depth and time. We will assume that there is a linear relationship between the partial pressure of CO_2 in the atmosphere, and the equilibrium concentration of DIC in seawater. Essentially what we are doing here is to apply Henry's law[4] directly to DIC, instead of applying it to the CO_2 and then finding the concentration of DIC from the details of the carbonate chemistry.

We know that the atmosphere currently contains approximately 415 ppm (by volume) of CO_2, which corresponds to a partial pressure of $p_{CO_2} = 415 \times 10^{-6}$ atm (assuming ideal gas). We also know that the sea surface concentration of dissolved inorganic carbon varies a bit, but is on average about $2.1 \,\mathrm{mol\,m^{-3}}$ (Wu et al., 2019, Fig. 1). From these points, and with the simplification described above, we get the following expression for the equilibrium concentration of DIC:

$$C_{eq} = H p_{CO_2}, \tag{4}$$

where $H = 5060 \,\mathrm{mol\,m^{-3}\,atm^{-1}}$ is a proportionality constant, similar to the constant in Henry's law.

Finally, to calculate the flux j_{mt} (Eq. (3)) we need the mass transfer coefficient, k_w. The mass transfer coefficient, k_w (units m/s), describes the change in the flux of CO_2 across the air-water interface, in response to a change in concentration. The mass transfer process is in reality quite complicated, and depends on a number of things, including temperature, and foam and bubbles created by waves. However, a common approach is to parameterise the mass transfer coefficient as a function of the wind speed, u. We will use the relationship

$$k_w = au^2, \tag{5}$$

where $a = 6.97 \times 10^{-7}$ s/m (Wanninkhof, 2014), and we will assume a constant average wind speed of 10 m/s, giving a mass transfer coefficient of 6.97×10^{-5} m/s.

3   Problems

This section describes the problems you should address in your report. First, you should briefly describe how you implemented your code, and any particular design choices you made. Then, you should complete all the tasks, and answer all the questions below. You do not need to repeat all the theory and information from this project description, but it may be helpful to refer to the description, for example when talking about specific equations.

You may hand in a report in pdf format, or a jupyter notebook. If you choose to hand in a notebook, make sure that you write enough text to explain what you have done, and answer all the questions. Please try to make the code clean and well commented, but you should also make sure that it is possible to read and understand your answers without reading any code. And make sure that all the figures are in place, so that the notebook makes sense without running the code.

Problem 1: Response to changing CO_2 concentration in shallow areas

One of the many concerns about the increasing amount of CO_2 in the atmosphere is that it leads to acidification of the ocean. As described in Section 2.2.2, CO_2 entering the ocean is stored as DIC, and one of the compounds included in DIC is H_2CO_3, which is an acid. If the pH of the oceans becomes too low, some species that depend on calcium carbonate shells may be unable to survive. This applies both to shellfish and some types of algae.

In this problem, we will consider a relatively shallow area, such as the Norwegian Continental shelf, and study approximately how long it takes for the water at the sea floor to respond to a change in the atmospheric concentration of CO_2. We want to find out if the concentration of DIC in the water "lags behind" the changes in the atmosphere, or if the whole water column is more or less at the equilibrium concentration predicted by the atmospheric CO_2.

We will look at an area where the water depth is $L = 100$ m. To represent the diffusivity at different depths, we will use the following expression:

$$K(z) = K_0 + K_a \frac{z}{z_a} \exp(-z/z_a) + K_b \frac{L-z}{z_b} \exp\left(-\frac{L-z}{z_b}\right), \tag{6}$$

$$K_0 = 10^{-3} \,\mathrm{m^2/s}, \quad K_a = 2 \times 10^{-2} \,\mathrm{m^2/s}, \quad z_a = 7\,\mathrm{m}, \quad K_b = 5 \times 10^{-2} \,\mathrm{m^2/s}, \quad z_b = 10\,\mathrm{m}.$$

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[4]https://en.wikipedia.org/wiki/Henry's_law

This expression has been chosen to approximately represent conditions where the water near the surface is influenced by wind, and the water near the bottom is influenced by friction of the current against the sea floor (see Fig. 1 in Visser (1997), and references therein for further details).

Tasks:

- At present, the concentration of CO_2 in the atmosphere is about 415 ppm, which is approximately equivalent to a partial pressure of 415×10^{-6} atm. Assume zero initial concentration of DIC in the ocean, and run a simulation for 180 days, using the diffusivity given by Eq. (6). The flux of CO_2 into the water is found from Eqs. (3)–(5).

- Plot the highest and lowest concentrations of DIC in the water column as a function of time, and see how they approach the equilibrium concentration.

- Plot also the concentration as a function of depth, for some different times, and discuss what you see.

- Considering that the level of CO_2 in the atmosphere changes only slowly from year to year (see Fig. 3), would you say that the water at 100 m depth is "in sync" with the changes in the atmosphere?

Problem 2: CO_2 absorption by the deep ocean

A key question in predicting how the climate responds to CO_2 emissions is to figure out how much CO_2 remains in the atmosphere, and how much is absorbed elsewhere. The main processes that remove CO_2 from the atmosphere are the growth of plants on land, and phytoplankton[5] in the ocean. Photosynthesis in the world's oceans consumes approximately 50×10^{15} g of carbon every year (Chavez et al., 2011), some of which is removed from circulation by sinking to the deep ocean floor when organisms die. However, also dissolution of CO_2 into the ocean acts as a sink for atmospheric carbon, since the increasing concentration of carbon in the ocean partially offsets the increase in the atmosphere.
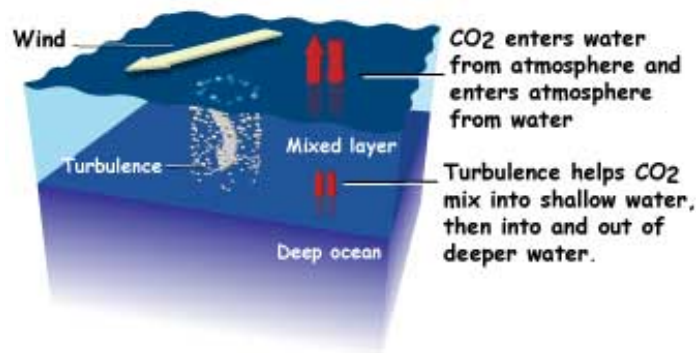

Figure 2: Mixing of CO_2 into the deeper ocean. Image source: NASA ClimateKids, `climatekids.nasa.gov/ocean/`.

In this problem, we will try to estimate the amount of CO_2 absorbed by the ocean on an annual basis. As above, we consider only mass transfer to bring atmospheric CO_2 into the surface waters, where it is transformed into DIC, and diffusion to mix the DIC down to greater depths. We will consider a water depth of 4000 m, which is approximately the average depth of the oceans as a whole. As an estimate of the diffusivity as a function of depth, we will use the function

$$K(z) = K_1 + \frac{K_0 - K_1}{1 + e^{-a(z-z_0)}},$$

$$K_0 = 10^{-4}\, m^2/s, \quad K_1 = 10^{-2}\, m^2/s, \quad a = 0.5\, m^{-1}, \quad z_0 = 100\, m.$$

(7)

This is a sigmoid function that gives a high diffusivity value, K_1, in the so-called surface mixed layer (see Fig. 2), and a low diffusivity value, K_0, in the deep ocean. Both the thickness of the mixed layer and the value of the diffusivity near the surface will in reality depend on local conditions, wind, time of year, etc. A value of $10^{-4}\, m^2/s$ for the deep ocean is also a simplification, but both theoretical considerations (Munk, 1966) and experimental studies (Rye et al., 2012) find values of about that order of magnitude.

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[5]Phytoplankton are all types of bacteria, algae, etc. in the ocean that obtain energy via photosynthesis.
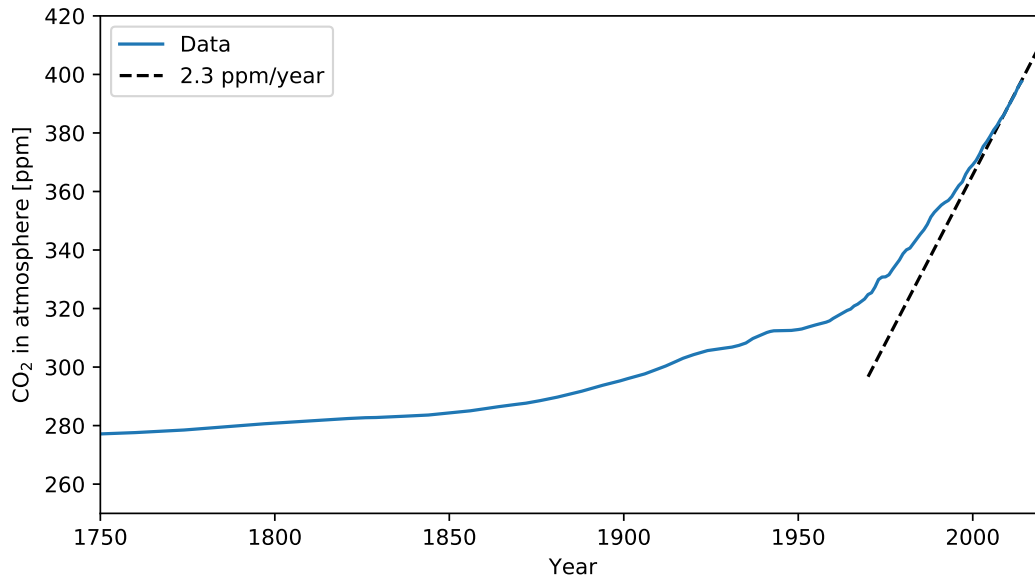
Figure 3: Concentration of CO_2 in the atmosphere over the past 270 years. The current growth rate of about $2.3\,\mathrm{ppm/year}$ is also shown.

Since the start of the industrial revolution, around 1750, the concentration of CO_2 in the atmosphere has been growing at an increasing rate, and at present the concentration is growing by about $2.3\,\mathrm{ppm/year}$, as shown in Fig. 3. In this problem, we are going to assume that the ocean is at present in equilibrium with the atmosphere, and then study the rate at which the ocean absorbs CO_2 as the concentration in the atmosphere keeps increasing.

Tasks:

- Assume that in the year 2020, the concentration of DIC (see Section 2.2.2) in the ocean was constant with depth, and in equilibrium with the atmospheric concentration of CO_2, which at the time was 415 ppm. Starting from this initial condition, run a siumlation for 10 years, until the year 2030, using a concentration of atmospheric CO_2 increasing by $2.3\,\mathrm{ppm/year}$, and the diffusivity given by Eq. (7).

- Plot the concentration as a function of depth, for the times 0, 2.5, 5 and 10 years into the simulation. Comment on the results, in light of the illustration in Fig. 2.

- Plot the total mass of DIC in the global oceans, as a function of time, for the years 2020–2030. The total area of the global oceans is $360 \times 10^{12}\,\mathrm{m}^2$, and the atomic mass of carbon is 12 grams per mole. We only count the mass of the carbon atoms, not the other elements involved. All of the DIC molecules and ions have exactly one atom of carbon each.

- Find the amount of CO_2 absorbed by the entire global ocean in a year by looking at the mass in the water column at the start of the simulation, compared to the mass at the end of the simulation, and take the average over the 10 years.

- Researchers have estimated that the oceans absorb so-called "anthropogenic CO_2" at a rate of about $2.5 \times 10^{15}\,\mathrm{g}$ per year (Gruber et al., 2019). Anthropogenic refers to CO_2 produced by human activities, and essentially means that they have calculated how much CO_2 the ocean absorbs *in addition* to what it would have done, had the CO_2 concentration remained at pre-industrial levels. Comment on how your answer relates to the number found by Gruber et al. (2019), in light of the simplifications we have made, and the number of processes we have ignored in formulating our model.

Appendix 1: Test cases

Before you start work on the other problems above, it is highly recommended to test your code on some cases with known results. Five such cases are described below. It is not necessary to include the test cases in your report.

Test case 1: The well-mixed condition

From Eq. (1), we can tell that if $\frac{\partial C(z,t)}{\partial z} = 0$ everywhere (and $K(z) > 0$) everywhere), then also the left-hand side of Eq. (1) will be zero, and hence nothing should happen. In other words, if the concentration is constant in space, it should remain constant for all time (even if $K(z)$ is not constant). This is known as the "well-mixed condition" (Thomson, 1987).

To test this, make sure you have no-flux boundary conditions at both boundaries, start out with $C(z, t = 0) = const$, and run the simulation for some time to ensure nothing happens.

Test case 2: Conservation of mass

If we use no-flux boundary conditions, then the mass in the system, given by

$$M = \int_0^L C(z,t)\, \mathrm{d}z, \tag{8}$$

should not change in time. This is called conservation of mass, and represents the fact that diffusion only redistributes mass, it does not create of destroy mass.

To test this, make sure you have no-flux boundary conditions at both boundaries, start out with some initial distribution, and run the simulation for some time (for example until the concentration starts approaching a constant value in space). Plot the difference between the initial mass, and the mass at later times, and see that it does not change too much (zero change is essentially impossible to achieve, due to the limited precision of floating point numbers in the computer).

Test case 3: Variance increases linearly in time

A fundamental properties of diffusion processes (with constant diffusivity) is that the variance, σ^2, of the distribution of the diffusing species increases linearly with time. Specifically, if you have a constant diffusivity, K, and an initial variance σ_0^2, then we have

$$\sigma^2 = \sigma_0^2 + 2Kt. \tag{9}$$

To test this, start with some initial distribution near the center of your system, far away from the boundaries, use a constant diffusivity, run the simulation for some time, and confirm that the variance as a function of time increases as expected. Note that this only holds in the absence of any boundaries. As soon as the distribution touches the boundaries, the variance will increase at a slower rate. The variance (also known as the central second moment) of the distribution is given by

$$\sigma^2 = \frac{\int_0^L C(z,t)(z-\mu)^2\, \mathrm{d}z}{\int_0^L C(z,t)\, \mathrm{d}z}, \tag{10}$$

where μ is the center of mass of the distribution (also known as the first moment), which is given by

$$\mu = \frac{\int_0^L C(z,t)\, z\, \mathrm{d}z}{\int_0^L C(z,t)\, \mathrm{d}z}. \tag{11}$$

Test case 4: Rate of mass transfer

A system that evolves with constant diffusion internally, and mass transfer at one boundary, can be described by a dimensionless number known as the mass-transfer Biot number, given by $\mathrm{Bi} = k_w L/K$, where L is the length of the system. The Biot number describes the relative speed of the mass transfer and the diffusion. If $\mathrm{Bi} \ll 1$, then diffusion is faster than the mass transfer, and as a consequence the concentration will remain approximately constant, because the diffusion will redistribute the mass to keep

an even concentration even as the mass transfer acts to change the concentration at the boundary. In the opposite case, when $\text{Bi} \gg 1$, then mass transfer is faster, and concentration will not remain even.

In this test case, we will consider the case where $\text{Bi} \ll 1$, and use this to reason about the dependence of mass transfer coefficient. If $\text{Bi} \ll 1$, then diffusion is fast enough to keep concentration approximately constant throughout the system. Hence, increasing the diffusivity, K, any further will not have an effect. Therefore, we conclude that the fate of the system depends only on the mass transfer. By dimensional analysis, we find that the product $\tau = L/k_w$ have units of time, and we may interpret this as the time scale for decay of the remaining mass.

To test this, set up a system with constant diffusivity, an initial concentration that is constant in space, one no-flux boundary and one mass-transfer boundary with 0 concentration outside (*i.e.*, set the flux through the boundary to be $j_{mt} = k_w C_0$ where C_0 is the concentration immediately inside the boundary). Make sure that your parameters correspond to $\text{Bi} \ll 1$. Simulate the system for some time, plot the remaining mass as a function of time, and compare to the theoretical decay given by

$$M(t) = M_0 \mathrm{e}^{-t\frac{k_w}{L}}. \tag{12}$$

Test case 5: Equilibrium concentration

In a system with CO_2 present in the atmosphere above water, the concentration of CO_2 in the water will eventually reach an equilibrium, where the concentration is constant in space, and has a value given by Henry's law (see Eqs. (3) and (4)). When this is the case, the flux predicted by Eq. (3) is equal to zero.

To test this, set up a system with some (positive) mass-transfer coefficient, and some (positive) diffusivity, initially zero concentration of CO_2 in the water, and a positive partial pressure of CO_2 in the air (this will remain constant in time). Run the simulation for some time, and confirm that the concentration approaches the value $C_{eq} = H p_{CO_2}$, for example by plotting both the maximum and the minimum concentration as a function of time. Note that the particular values of k_w and $K(z)$ do not affect the equilibrium concentration, but they *will* affect the time it takes to reach equilibrium.

Appendix 2: Numerical scheme for the diffusion equation

The diffusion equation (Eq. (1)) is a PDE that involves partial derivatives with respect to both space and time. Hence, we need a way do express these numerically. We start by discretising space and time:

$$z_n = z_0 + n\Delta z, \quad t_i = t_0 + i\Delta t, \tag{13}$$

where i and n are integers, and specifically $n \in \{0, 1, 2, \ldots, N\}$, such that we have in total $N + 1$ points in space. Furthermore, we will use the shorthand notation

$$C_n^i = C(z_n, t_i), \quad K_n = K(z_n) \tag{14}$$

Next, we rewrite Eq. (1) slightly, and get

$$\frac{\partial C(z,t)}{\partial t} = K(z)\left(\frac{\partial^2 C(z,t)}{\partial z^2}\right) + \left(\frac{\partial K(z)}{\partial z}\right)\left(\frac{\partial C(z,t)}{\partial z}\right). \tag{15}$$

Starting with space, we will use finite-difference approximations of the derivatives:

$$\frac{\partial f(z,t)}{\partial z} \approx \frac{f(z+\Delta z, t) - f(z - \Delta z, t)}{2\Delta z} \tag{16a}$$

$$\frac{\partial^2 f(z,t)}{\partial z^2} \approx \frac{f(z+\Delta z, t) - 2f(z,t) + f(z-\Delta z, t)}{\Delta z^2} \tag{16b}$$

Inserting this into Eq. (15), and using the shorthand notation defined above, we get

$$\frac{\partial C(z,t)}{\partial t} \approx K_n \frac{C_{n+1}^i - 2C_n^i + C_{n-1}^i}{\Delta z^2} + \frac{K_{n+1} - K_{n-1}}{2\Delta z}\frac{C_{n+1}^i - C_{n-1}^i}{2\Delta z} \tag{17}$$

This is sometimes called the semi-discretised form of the PDE, and it is essentially a set of coupled ODEs, which tell us how the concentration at each point will change in time. To integrate this equation in time, we will use the Crank-Nicolson method (see Section 8.1.4 in the textbook by Sauer). This method says

$$C_n^{i+1} = C_n^i + \Delta t \frac{1}{2}\big(F(z_n, t_i) + F(z_n, t_{i+1})\big), \tag{18}$$

where F represents the right-hand side of the PDE. Since the right-hand side of the PDE is equal to the time derivative, the Crank-Nicolson method essentially says that to find the value at the next timestep, C_n^{i+1}, we take the value at the current timestep and add an increment that we find by multiplying the timestep, Δt, with the average of the right-hand side at present and at the next timestep. This means that we have to solve an equation to find C_n^{i+1}, making this an implict method.

Inserting our semi-discretised equation into Eq. (18), we get

$$C_n^{i+1} = C_n^i + \Delta t \frac{1}{2}\left[K_n \frac{C_{n+1}^{i+1} - 2C_n^{i+1} + C_{n-1}^{i+1}}{\Delta z^2} + \frac{K_{n+1} - K_{n-1}}{2\Delta z} \frac{C_{n+1}^{i+1} - C_{n-1}^{i+1}}{2\Delta z} \right.$$
$$\left. + K_n \frac{C_{n+1}^i - 2C_n^i + C_{n-1}^i}{\Delta z^2} + \frac{K_{n+1} - K_{n-1}}{2\Delta z} \frac{C_{n+1}^i - C_{n-1}^i}{2\Delta z} \right]. \tag{19}$$

Now we just have one problem left, and that is that the equation for the concentration at the surface, C_0 is expressed in terms of C_{-1}, which is outside our domain, and similarly the concentration at the sea floor, C_N is expressed in terms of C_{N+1}, which is also outside our domain. Mathematically speaking, we have $N + 3$ unknowns, but only $N + 1$ equations. Hence, we need to eliminate the two unwanted unknowns. To do this, we will use Fick's law (Eq. (2)), and our knowledge of the fluxes at the boundaries.

If we express Fick's law in terms of the finite difference approximation of the derivative, we get

$$j_D(z_n) = -K(z_n)\frac{\partial C(z,t)}{\partial z}\Bigg]_{z_n} \approx K_n \frac{C_{n+1}^i - C_{n-1}^i}{2\Delta z}. \tag{20}$$

Starting with the sea floor, at position z_N, we said that there the flux would be 0. Hence, we get

$$j_D(z_N) \approx K_N \frac{C_{N+1}^i - C_{N-1}^i}{2\Delta z} = 0 \Rightarrow C_{N+1} = C_{N-1}. \tag{21}$$

For the sea surface, we take the same approach, except that here the flux is not 0, but given by Eq. (3):

$$j_D(z_0) \approx K_0 \frac{C_1^i - C_{-1}^i}{2\Delta z} = -k_w\left(C_0 - C_{eq}\right) \Rightarrow C_{-1} = C_1 + \frac{2\Delta z k_w}{K_0}\left(C_0 - C_{eq}\right). \tag{22}$$

Now we have everything we need to proceed with the implementation. To do so, we are going to express our numerical scheme as a matrix equation, of the form

$$\mathbf{L}\mathbf{C}^{i+1} - \frac{1}{2}\mathbf{S}^{i+1} = \mathbf{R}\mathbf{C}^i + \frac{1}{2}\mathbf{S}^i, \tag{23}$$

where $\mathbf{L}$ and $\mathbf{R}$ are tridiagonal $(N+1) \times (N+1)$ matrices, $\mathbf{C}^i$ and $\mathbf{C}^{i+1}$ are column vectors with $N+1$ elements, giving the concentration at each point in space (for times t_i and t_{i+1} respectively), and $\mathbf{S}^i$ is a $N+1$ component vector with only one non-zero element, which is responsible for the flux at the surface. The non-zero element is the first, such that $\mathbf{S}^i$ is given by

$$\mathbf{S}^i = \left[2\Gamma C_{eq}^i, 0, 0, 0, \cdots, 0\right]^{\mathrm{T}}, \tag{24}$$

where the superscript T indicates that it should be transposed into a column vector. Note that in $\mathbf{S}^i$, the variable C_{eq}^i is the equilibrium concentration at time t_i. In Problem 1, the equilibrium concentration is constant in time, while in Problem 2, it will change with time, as given by the concentration of CO_2 in the atmosphere, and Eq. (4).

You can obtain $\mathbf{L}$ and $\mathbf{R}$ yourself, from Eqs. (19), (21) and (22), but for your convenience they are given below. In Eqs. (24) and (26) we have used the following shorthand[6] (to make the matrices fit on the page):

$$\alpha = \frac{\Delta t}{2\Delta z^2}, \quad K_n' = K_{n+1} - K_{n-1}, \quad \Gamma = 2\alpha k_w \Delta z\left(1 - \frac{K_1 - K_0}{2K_0}\right). \tag{25}$$

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[6]For those of you who are wondering: In Γ, we have used a one-sided finite difference to approximate the derivative of $K(z)$, to avoid using the value in a point outside the domain.

$$\mathbf{L} = \begin{pmatrix} 1+2\alpha K_0 + \Gamma & -2\alpha K_0 & 0 & & & 0 & & 0 \\ \frac{\alpha}{4}K_1' - \alpha K_1 & 1+2\alpha K_1 & -\frac{\alpha}{4}K_1' - \alpha K_1 & 0 & & & & 0 \\ 0 & & & & & 0 & & \\ & 0 & \frac{\alpha}{4}K_n' - \alpha K_n & 1+2\alpha K_n & -\frac{\alpha}{4}K_n' - \alpha K_n & 0 & & \\ & & 0 & & & & & 0 \\ 0 & & & 0 & \frac{\alpha}{4}K_{N-1}' - \alpha K_{N-1} & 1+2\alpha K_{N-1} & -\frac{\alpha}{4}K_{N-1}' - \alpha K_{N-1} \\ 0 & & 0 & & & 0 & -2\alpha K_N & 1+2\alpha K_N \end{pmatrix} \quad (26\text{a})$$

$$\mathbf{R} = \begin{pmatrix} 1-2\alpha K_0 - \Gamma & 2\alpha K_0 & 0 & & & 0 & & 0 \\ -\frac{\alpha}{4}K_1' + \alpha K_1 & 1-2\alpha K_1 & \frac{\alpha}{4}K_1' + \alpha K_1 & 0 & & & & 0 \\ 0 & & & & & 0 & & \\ & 0 & -\frac{\alpha}{4}K_n' + \alpha K_n & 1-2\alpha K_n & \frac{\alpha}{4}K_n' + \alpha K_n & 0 & & \\ & & 0 & & & & & 0 \\ 0 & & & 0 & -\frac{\alpha}{4}K_{N-1}' + \alpha K_{N-1} & 1-2\alpha K_{N-1} & \frac{\alpha}{4}K_{N-1}' + \alpha K_{N-1} \\ 0 & & 0 & & & 0 & 2\alpha K_N & 1-2\alpha K_N \end{pmatrix} \quad (26\text{b})$$

Iteration through time

In your program, you should first construct the matrices $\mathbf{L}$ and $\mathbf{R}$. These remain constant, so they only have to be constructed once. At every timestep (including the first), we start out knowing the concentration at every point, at the current time, which is given by the components of the column vector $\mathbf{C}^i$. In order to calculate the concentration in every point, at the next time, $\mathbf{C}^{i+1}$, we first find the vector

$$\mathbf{V} = \mathbf{R}\mathbf{C}^i + \frac{1}{2}\left(\mathbf{S}^i + \mathbf{S}^{i+1}\right). \quad (27)$$

Then we solve the following system of linear equations to find $\mathbf{C}^{i+1}$:

$$\mathbf{L}\mathbf{C}^{i+1} = \mathbf{V}, \quad (28)$$

Since $\mathbf{L}$ and $\mathbf{R}$ are tridiagonal, it is not strictly necessary to store all the elements of the matrices, as the vast majority of the elements are 0. Storing the three diagonals will suffice. You can either do this "manually", by creating three 1D arrays, or you can make use of a sparse array structure, such as `scipy.sparse.dia_matrix`. Using an existing sparse array structure requires you to read a little bit of documentation, but it has the added convenience that the method for calculating the matrix-vector product you need in Eq. (27) is built in.

To solve the linear system of equations in Eq. (28), we can again make use of the fact that $\mathbf{L}$ is tridiagonal. The tridiagonal matrix algorithm (TDMA), also known as the Thomas algorithm, is a fast and simple approach for solving such systems. You may find it described for example in (Quarteroni et al., 2000, p. 97), and you will find a python implementation and some description at `http://folk.ntnu.no/leifh/teaching/tkt4140/._main040.html`. You will also find an implementation of the TDMA in a notebook in the folder for Project 1 on Blackboard.

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