Mass and Heat Transfer

Assigment 1 | MNI 2

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Contents

Problem Context

In this homework exercise we must solve the one-dimensional advection-diffusion equation below, for species i:

$$\frac{\partial \rho}{\partial t} = D_{ij} * \frac{\partial^2 \rho}{\partial x^2} - v_x \frac{\partial \rho_i}{\partial x} \quad (1)$$

With:

- D_{ij} the binary diffusion coefficient of species I through species j;
- v_x the constant mass average velocity of the binary fluid mixture;

Initial condition:

- the mass concentration of species i is equal to ρ_{i0}

Boundary conditions:

- at $x = 0,\ \rho_i(0, t) = \rho_{imax}$,$\forall t > 0$
- at $x = L,\ \rho_i(L, t) = \rho_{i0}$,$\forall t$

1 Discretization

We will use a Finite difference scheme and be at the generic node I.

- The spatial discretization will equal to:

$$\Delta x = \frac{L}{N}$$

With N the mesh size (N=number of nodes-1)

- The temporal discretization will equal to:

$$\Delta t = \frac{T}{N_t}$$

With N_t the number of time steps and T the total time

- We use a Euler discretization method for time:

$$\frac{\partial \rho}{\partial t} = \frac{\rho_i(x, t + \Delta) - \rho_i(x, t)}{\Delta t} = \frac{\rho_{iI}^{n+1} - \rho_{iI}^{n}}{\Delta t} \quad (2)$$

- Upstream finite difference scheme:

$$\frac{\partial \rho_i}{\partial x} = \frac{\rho_i(x, \blacksquare) - \rho_i(x - \Delta x, \blacksquare)}{\Delta x} = \frac{\rho_{iI}^{\blacksquare} - \rho_{iI-1}^{\blacksquare}}{\Delta x} \quad (3)$$

➢ Central finite difference scheme:

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\rho_i(x+\Delta x, ■) - 2\rho_i(x, ■) - \rho_i(x-\Delta x, ■)}{\Delta x^2} = \frac{\rho_{iI+1}^{■} - 2\rho_{iI}^{■} - \rho_{iI-1}^{■}}{\Delta x^2} \quad (4)$$

By introducing discretized equations (2), (3) and (4) into the equation (1), we have the equation below:

$$\frac{\rho_{iI}^{n+1} - \rho_{iI}^{n}}{\Delta t} = D_{ij} * \frac{\rho_{iI+1}^{■} - 2\rho_{iI}^{■} - \rho_{iI-1}^{■}}{\Delta x^2} - v_x * \frac{\rho_{iI}^{■} - \rho_{iI-1}^{■}}{\Delta x} \quad (5)$$

2 Numerical Model

Using a Fully Euler implicit scheme we will be at time T^{n+1} and at node I. The equation (5) will transform as below:

$$\frac{\rho_{iI}^{n+1} - \rho_{iI}^{n}}{\Delta t} = D_{ij} * \frac{\rho_{iI+1}^{n++1} - 2\rho_{iI}^{n+1} - \rho_{iI-1}^{n+1}}{\Delta x^2} - v_x * \frac{\rho_{iI}^{n+1} - \rho_{iI-1}^{n+1}}{\Delta x} \quad (6)$$

By separating all the time T^{n+1} and T^{n} terms, we obtain:

$$(-\Delta t \Delta x v_x - \Delta t D_{ij})\rho_{iI-1}^{n+1} + \left(v_x \Delta t \Delta x + 2D_{ij}\Delta t + \Delta x^2\right)\rho_{iI}^{n+1} + \left(-\Delta t D_{ij}\right)\rho_{iI+1}^{n++1} = \Delta x^2 \rho_{iI}^{n} \quad (7)$$

$$\leftrightarrow a * \rho_{iI-1}^{n+1} + b * \rho_{iI}^{n+1} + c * \rho_{iI+1}^{n++1} = d * \rho_{iI}^{n} \quad (8)$$

Avec:

$$\begin{cases} a = (-\Delta t \Delta x v_x - \Delta t D_{ij}) \\ b = \left(v_x \Delta t \Delta x + 2D_{ij}\Delta t + \Delta x^2\right) \\ c = \left(-\Delta t D_{ij}\right) \\ d = \Delta x^2 \end{cases} \quad (9)$$

We can thus form the following matrix:

$$\begin{bmatrix} b & c & 0 & \cdots & \cdots & 0 \\ a & b & \ddots & \ddots & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & c \\ 0 & \cdots & \cdots & 0 & a & b \end{bmatrix} \begin{bmatrix} \rho_{i1}^{n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \rho_{iN-1}^{n+1} \end{bmatrix} = \begin{bmatrix} d\rho_{i1}^{n} - a\rho_{i0}^{n} \\ d\rho_{i2}^{n} \\ \vdots \\ \vdots \\ d\rho_{N-2}^{n} \\ d\rho_{iN-1}^{n} - c\rho_{iN}^{n} \end{bmatrix} \quad (10)$$

$$\leftrightarrow A * X = B \text{ with } X \text{ the unknown matrix}$$

For each time step, we will solve the matrix equation (10) using a tridiagonal matrix system solver. The result is written in the code in the file “advection-diffusion.f90”.

3 Pure diffusive transport

In a pure diffusive transport $v_x = 0\ m/s$ and the equation (1) becomes the equation below:

$$\frac{\partial \rho}{\partial t} = D_{ij} * \frac{\partial^2 \rho}{\partial x^2} \ (1.1)$$

The analytical solution of this equation in a semi-infinite stationary liquid is given in our Heat and mass transfer courses[1]:

$$\frac{\rho_i - \rho_{i0}}{\rho_{imax} - \rho_{i0}} = 1 - \mathrm{erf}\left(\frac{x}{2 * \sqrt{D_{ij} t}}\right) \ (11)$$

If we take $\rho_{i0} = 0$ then (11) becomes:

$$\rho_i = \rho_{imax} - \rho_{imax} * \mathrm{erf}\left(\frac{x}{2 * \sqrt{D_{ij} t}}\right) \ \ (12)$$

In the Figure 1 below, we can see a plot of the analytical solution and the results of our numerical model. We have taken L=3 to for the semi-infinite condition.

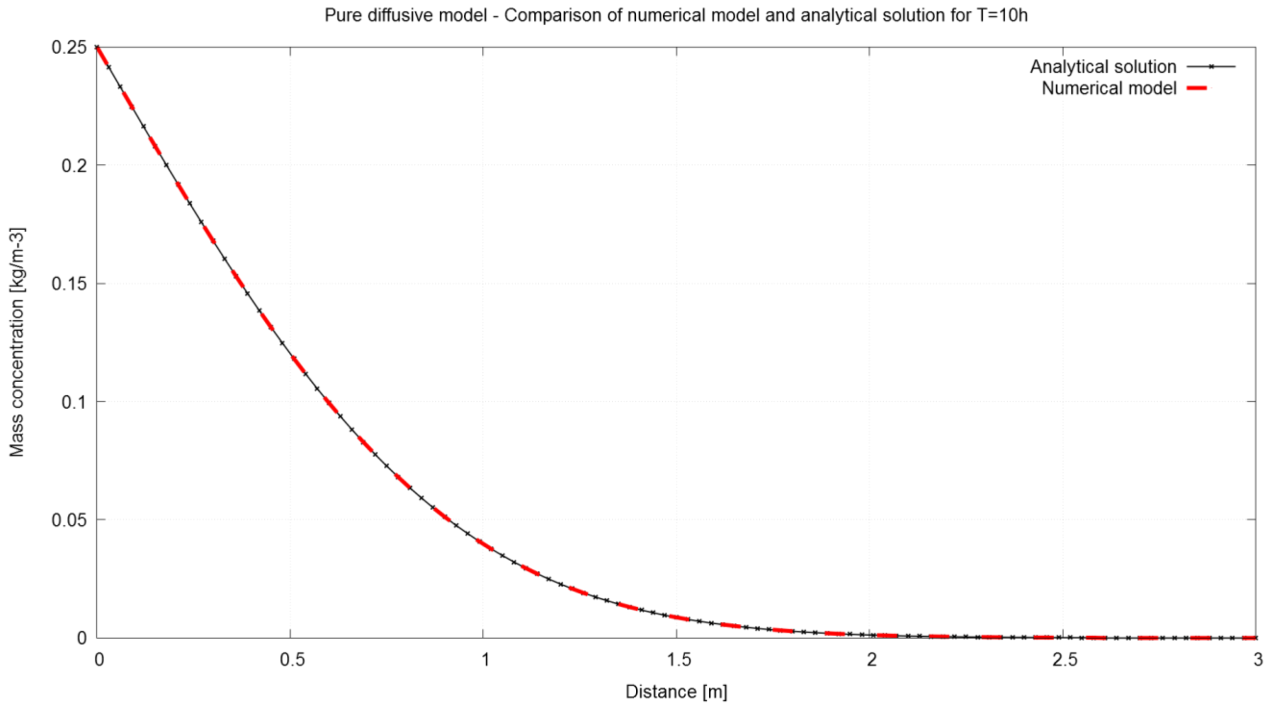

Figure 1: Pure diffusive model

$$L = 3\mathrm{m}, v_x = 0\ \mathrm{m/s}, D_{ij} = 7 * 10^{-6}\ \mathrm{m^2/s}\ , \rho_{i0} = 0\ \mathrm{kg/m^3}, \rho_{imax} = 0.25\ \mathrm{kg/m^3}$$

[1] Heat and mass transfer courses. G.Schäfer. 2013/2014

Conclusion:

The analytical solution shows us that the mass concentration spread toward the right side of the domain where the mass concentration is lower. With our Fortran model we observe the same phenomenon and the curves obtained are nearly the same. Hence, we can say that our Fortran model is accurate for pure diffusive transport.

4 Pure advective transport

We choose this time to model a pure advective transport, hence $D_{ij} = 0\, m^2/s$ and the equation (1) becomes the equation :

$$\frac{\partial \rho}{\partial t} = -v_x \frac{\partial \rho_i}{\partial x} \ (1.2)$$

Impact of time discretization:

There can be instability problems in regions were the advection is dominant. To remediate at these problems, we can reduce the time step.

- Since we have used a fully implicit scheme upstream and central method, Δt can take any value and the scheme will always be stable. Hence we can take a big Δt to decrease the calculation time. However if we had taken a downstream discretization the scheme will be stable for :

$$Pe = \frac{v_x * \Delta x}{D} < 2 \ \ (13)$$

- Contrariwise, if we had taken an fully explicit scheme, the Δt should have respected the CFL[2] criterion of stability.

$$CFL = v_x \frac{\Delta t}{\Delta x} \leq 1 \ \ (14)$$

[2] Courant–Friedrichs–Lewy criterion

We have plotted in the Figure 2 below the pure advective model with different time-step.

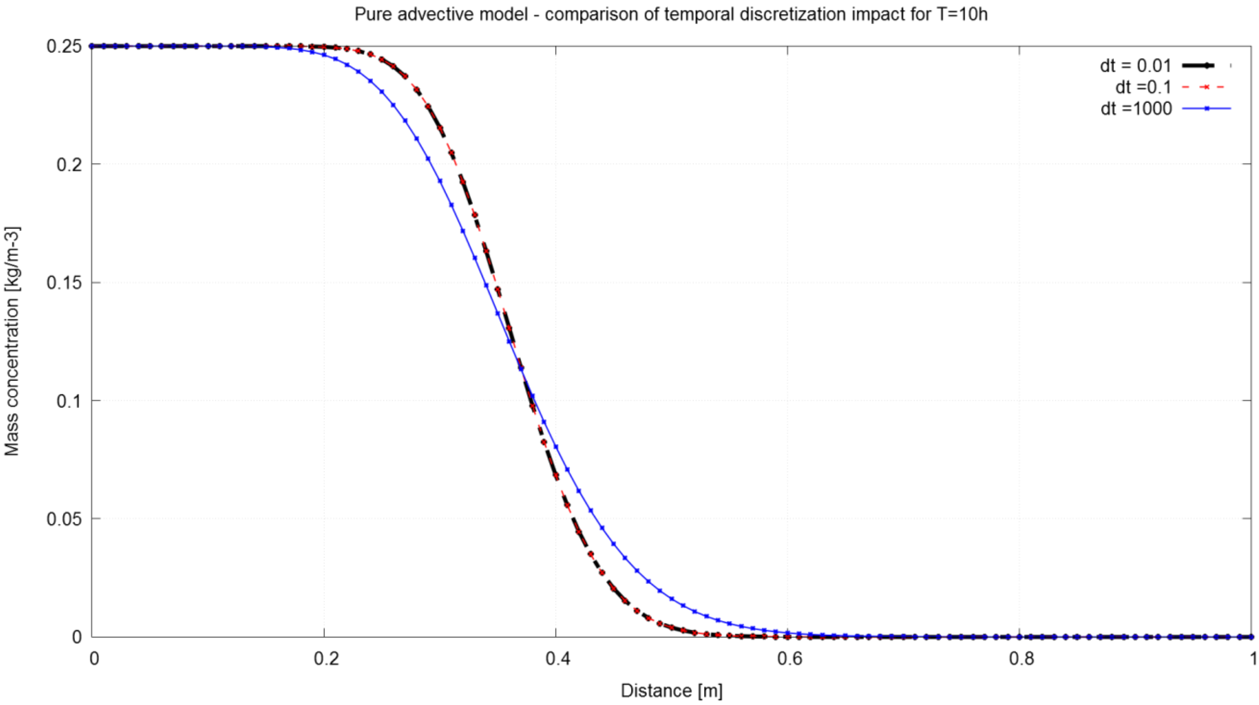

Figure 2: Pure advective model – Time discretization impact

$$L = 1\text{m}, v_x = 10^{-5}\ \text{m/s}, D_{ij} = 0\ \text{m}^2/\text{s}\ , \rho_{i0} = 0\ \text{kg/m}^3, \rho_{imax} = 0.25\ \text{kg/m}^3$$

We can see, as we have used a fully implicit scheme upstream and central method, that the different time step does not change the mass concentration. We have to take a high time step (dt=1000) to see a change in the results.

Impact of spatial discretization:

We have used a finite difference method. Thus to obtain an acceptable numerical scheme the numerical diffusion has to be much lower than a physical diffusion D, thus we grid that we use Δx must respect the equation below:

$$Pe \ll 2 \ \ (15)$$

Thus criterion oblige us in case of large model to have a use number of cells, limiting the use of the finite difference method.

In our case we have : $Pe = \frac{10^{-5} * (\frac{1}{100})}{7 * 10^{-6}} = 0.014 \ll 2$. We respect the criterion (15).

We have plotted in the Figure 3 below the pure advective model with different size of meshes.

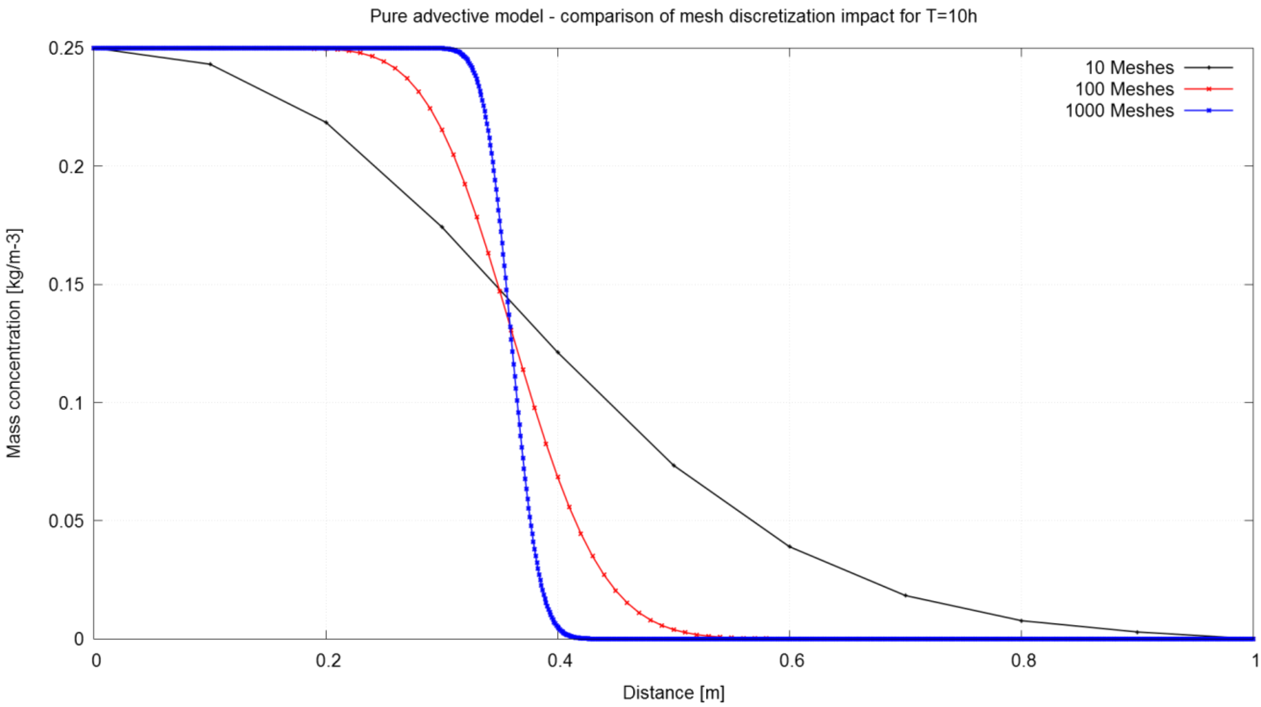

Figure 3: Pure advective model – Space discretization impact

$$L = 1\text{m}, v_x = 10^{-5}\ \text{m/s}, D_{ij} = 0\ \text{m}^2/\text{s}\ , \rho_{i0} = 0\ \text{kg/m}^3, \rho_{imax} = 0.25\ \text{kg/m}^3$$

We can see that the mesh size has a large influence on the mass concentration. Hence, with a 10 meshes size, we don't respect the criterion (15) and the result obtain has a high marge of error.

5 Diffusion and advection transport

Calculation of the mass concentration at T=5 and 10 hours, with:

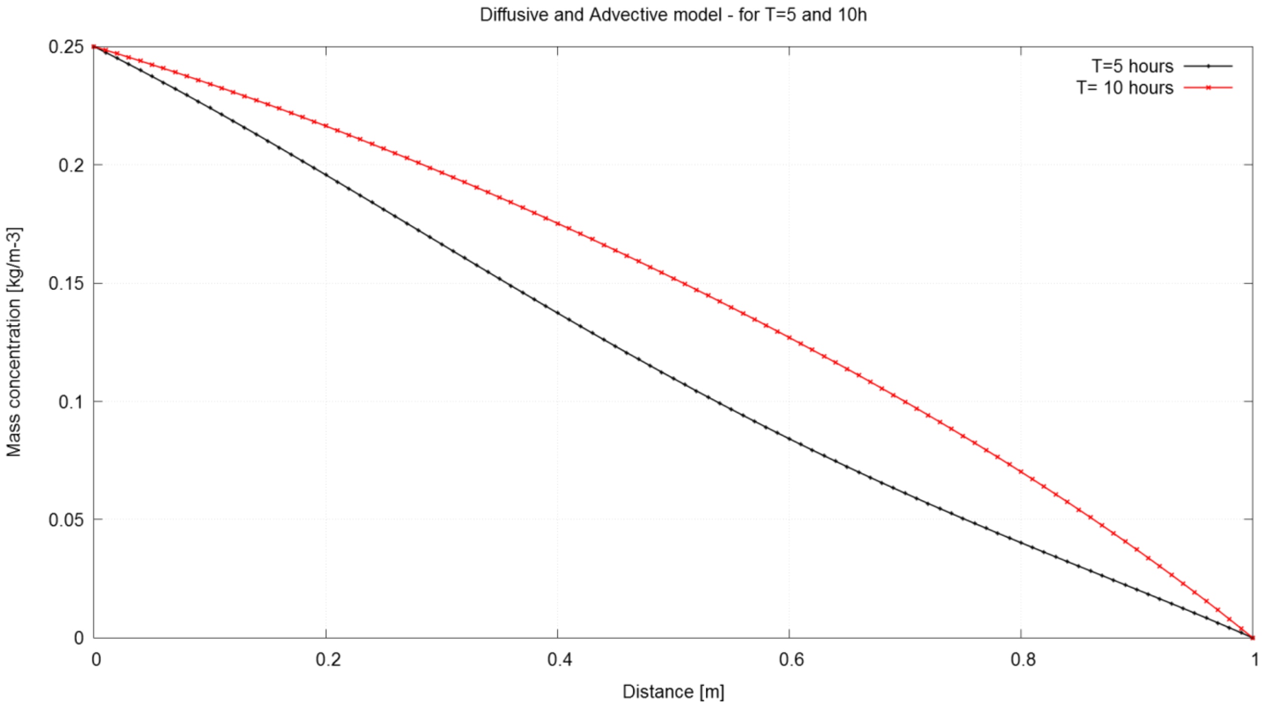

Figure 4: Diffusive and advective model

$$L = 1\text{m}, v_x = 10^{-5}\ \text{m/s}, D_{ij} = 7 * 10^{-6}\ \text{m}^2/\text{s}\ , \rho_{i0} = 0\ \text{kg/m}^3, \rho_{imax} = 0.25\ \text{kg/m}^3$$

6 Coupled flow and transport model (gaz phase)

We want here to calculate a one dimensional TCE vapor mass transfer in a partially water saturated homogeneous porous medium.

$$S_a \varepsilon \frac{\partial C_a}{\partial t} = \frac{\partial}{\partial z}(D_a^{eff} * \frac{\partial C_a}{\partial z}) - \frac{\partial}{\partial z}(S_a \varepsilon v_a C_a) \quad (16)$$

We want solve this equation. But unlike the equation (1), here v_a is not constant and depends on P_a that is itself dependent of ρ_a, that depends on C_a. Hence we must calculate the gas density via the equation below:

$$\rho_a = C_{a(old)} \left(1 - \frac{M_{air}}{M_{TCE}}\right) + \rho_{air} \quad (17)$$

Then we can solve the flow equation for density-dependent gas flow that can be written as follows to obtain P_a:

$$\frac{\partial}{\partial z}\left(\frac{k_{ra}k^{*}\rho_a}{\mu_a}\left(\frac{\partial P_a}{\partial z}+\rho_a g\right)\right)=S_a\varepsilon\frac{\partial \rho_a}{\partial t}\ (18)$$

We can then calculate the average pore velocity of the gas flow with the equation below:

$$v_a=-\frac{k_{ra}k^{*}\rho_a}{\mu_a S_a\varepsilon}(P_a+\rho_a gz)\ (19)$$

Hence we will be able to solve the equation (16) and to obtain a new C_a:

$$S_a\varepsilon\frac{\partial C_{a(new)}}{\partial t}=\frac{\partial}{\partial z}(D_a^{eff}*\frac{\partial C_{a(new)}}{\partial z})-\frac{\partial}{\partial z}(S_a\varepsilon v_a C_{a(new)})\ (20)$$

For the next time step we will do $C_{a(old)}=C_{a(new)}$ and thus we will be able to calculate the equation (17) , (18) , (19) and (20).

We can summarize this with the simplified flow chart below: