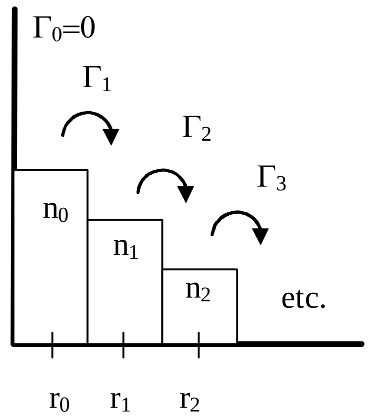
Diffusion in cylindrical geometry



In this exercise we will solve the diffusion equation in cylindrical geometry. We will use the same approach that was used for planar geometry.
The continuity equation with a source term is

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma} = S$$ which, for cylindrical symmetry is:

$$\frac{\partial n}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\Gamma) = S$$

where S is the source term and Γ(r,t) is the radial flux of particles.

Fick's law, in cylindrical geometry is:

$$\Gamma = -D\frac{\partial n(r,t)}{\partial r}$$ where D is the diffusivity.

These equations will be solved in finite-difference form by iteration.
The continuity equation becomes:

$$\frac{n(r+\frac{1}{2}\Delta r, t+\Delta t) - n(r+\frac{1}{2}\Delta r, t)}{\Delta t} + \frac{1}{r}\frac{\left[(r+\Delta r)\Gamma(r+\Delta r, t) - r\Gamma(r,t)\right]}{\Delta r} = S$$

where n(r,t) is defined on half-grid points $r_m+\Delta r/2$, and Γ(r,t) is defined on grid points r_m.
The reason for half grid points is that it makes the **derivative** of Γ centered at the points at which n(r,t) is evaluated. This can be rearranged to find n at the next time step in terms of the previous value of n and the fluxes:

$$n(r+\tfrac{1}{2}\Delta r, t+\Delta t) = n(r+\tfrac{1}{2}\Delta r, t) - \frac{\Delta t}{\Delta r}\frac{\left[(r+\Delta r)\Gamma(r+\Delta r, t) - r\Gamma(r,t)\right]}{r} + S\Delta t$$

Γ is found from the finite difference form of Fick's law:

$$\Gamma(r,t) = -\frac{D}{\Delta r}\left[n(r+\tfrac{1}{2}\Delta r, t) - n(r-\tfrac{1}{2}\Delta r, t)\right]$$

This equation also has the number density evaluated at half grid points. The continuity equation and Fick's law may be combined to give the diffusion equation in cylindrical geometry:

$$\frac{\partial n}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial n}{\partial r}\right) + S$$

In this exercise, we will solve simultaneously the continuity equation and Fick's law which is equivalent to solving the diffusion equation.

The r grid:

We will divide the r axis into cells with boundaries at multiples of Δr. Each cell is a ring with area $2\,\pi\,r\,\Delta r$. Γ_m is the flux density of particles entering cell (m,m+1) at the left boundary.

Γ_{m+1} is the flux density of particles leaving cell (m,m+1) at the right boundary and entering the next cell. Cell (m, m+1) is centered at $r_m + \Delta r/2$ and the number density n_m is the number density at the center of the cell.

$R := 5$ The radius of the cylindrical volume. R is also the center of cell (mmax-1,mmax).

$mmax := 10$ mmax + 1 is the number of r grid points

We will put the center of the cells at half grid points and the cell boundaries at grid points. The center of the last cell, where the density is set to zero, is the plasma boundary, r = R.

$m := 0..mmax \quad r_m := R\cdot\frac{m+0.5}{mmax+0.5} \qquad \Delta r := r_1 - r_0 \qquad \Delta r = 0.476$

$D := 1$ is the diffusivity.

$tDiff := \frac{2}{D}\left(\frac{R}{2.405}\right)^2$ tDiff is the analytic solution for the characteristic decay time. 2.405 is the first root of the zeroth Bessel function, which is the lowest order analytic solution for the cylindrical diffusion equation.

$tmax := 2\cdot tDiff$ We will perform interations for two diffusion times.

The time step Δt needed for stability is approximately the diffusion time across one grid cell:

$\Delta t := \frac{\Delta r^2}{2\cdot D} \qquad \Delta t = 0.113$ Approximate number of time steps: $Tsteps := \frac{tmax}{\Delta t}$

$Tsteps = 152.489$ Make Tsteps an integer divisible by four to make the final plot nicer:

$jmax := 4\cdot ceil\left(\frac{Tsteps}{4}\right) \qquad jmax = 156 \qquad \Delta t := \frac{tmax}{jmax} \qquad \Delta t = 0.111 \qquad j := 0..jmax$

jmax is the number of time steps we need if we integrate numerically for two diffusion times.

Using symmetry:

We assume that our problem is symmetric about the axis. The density will be peaked on the axis, to the left of grid point zero. We will use an initial profile that is the zero order Bessel function, J0(r). There is no flux across the midplane because the first derivative of the density is zero (see Fick's law). The density profile is a maximum at the origin and is zero at the center of the last cell.

The initial density profile n0 that we will use is the Bessel function profile that is the analytic solution to the diffusion equation in cylindrical geometry.

$$n0_m := J0\left(2.4048\cdot\frac{r_m}{R}\right)$$

Because there is no flux across the midplane, $\Gamma_0 = 0$. Γ_0 is shorthand notation for Γ entering the zeroth cell. The particles lost from the cylinder are lost at the left side of the cell numbered mmax thus the losses from the system are 2π (mmax Δr) Γ_{mmax} summed for each time step, where 2π (mmax Δr) is the circumference where Γ_{mmax} is evaluated. Γ is a particle flux density, thus we must multiply Γ by the circumference to get the loss rate of particles.

Particle conservation:
The number of particles in the last cell is zero, because this is a boundary condition, even though particles enter the cell from the left. Thus the particles entering the last cell from the left are the particles that are lost.
The source term S is the number of particles created per unit area (of the cross section) per unit time. Thus the number of particles added to the system to the left of the last cell is $S\,\pi\,(\mathrm{mmax}\,\Delta r)^2\,\mathrm{jmax}\,\Delta t$. The number of particles lost per unit time is $2\pi(\mathrm{mmax}\,\Delta r)\Gamma_{mmax}$. The sum of $2\pi(\mathrm{mmax}\,\Delta r)\Gamma_{mmax}\,\Delta t$ at every time step is the total number of particles lost. We have conserved particles if the **final** number of particles minus the **initial** number of particles is equal to the **gain** in particles minus the **loss** in particles.

$S := 0$ We will begin with no source of new particles. The program loop is:

$$
M(n0,S) := \left|\begin{array}{l}
M_{jmax,mmax} \leftarrow 0 \\
\Gamma_{mmax} \leftarrow 0 \\
\text{for } m \in 0..\mathrm{mmax} \\
\quad M_{0,m} \leftarrow n0_m \\
\text{for } j \in 1..\mathrm{jmax} \\
\quad \left|\begin{array}{l}
\text{for } m \in 1..\mathrm{mmax} \\
\quad \Gamma_m \leftarrow -\dfrac{D}{\Delta r}\cdot\left(M_{j-1,m} - M_{j-1,m-1}\right) \\
\text{for } m \in 0..\mathrm{mmax}-1 \\
\quad M_{j,m} \leftarrow M_{j-1,m} + \dfrac{1}{r_m}\cdot\dfrac{\Delta t}{\Delta r}\cdot\left[\left(r_m - \dfrac{\Delta r}{2}\right)\cdot\Gamma_m - \left(r_m + \dfrac{\Delta r}{2}\right)\cdot\Gamma_{m+1}\right] + S\cdot\Delta t
\end{array}\right. \\
M
\end{array}\right.
$$

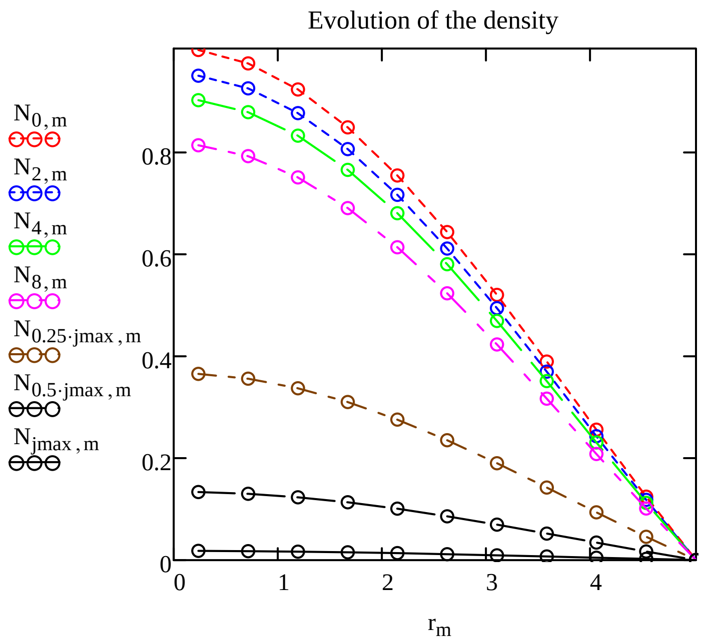
At each time step j, the fluxes Γ_m are calculated within a for loop. The following loop "updates" the values of the densities (stored in M) using the fluxes.
The loop does not change $M_{j,mmax}$, thus the boundary conditions at r = R are preserved.

As we go down the first column, we see the decay in the central density.

$M(n0,S) =$

	0	1	2	3	4	5	6	7	8	9	10
0	1	0.97	0.92	0.85	0.75	0.64	0.52	0.39	0.25	0.12	$\ldots\cdot 10^{-5}$
1	0.97	0.95	0.9	0.82	0.73	0.62	0.5	0.38	0.25	0.12	0
2	0.95	0.92	0.87	0.8	0.71	0.61	0.49	0.37	0.24	0.12	0
3	0.92	0.9	0.85	0.78	0.7	0.59	0.48	0.36	0.24	0.11	0
4	0.9	0.88	0.83	0.76	0.68	0.58	0.47	0.35	0.23	0.11	0
5	0.88	0.85	0.81	0.74	0.66	0.56	0.46	0.34	0.22	0.11	0
6	0.85	0.83	0.79	0.72	0.64	0.55	0.44	0.33	0.22	0.11	...

$N := M(n0, S)$ M(n0,S) was made a function so that we could change n0 or S without typing again the program loop. If we convert M from a function to a fixed matrix N, the regions below compute faster.



Question:
Is the central density e^{-2} of the starting density after the two decay times?

Demonstration of particle conservation:

$$\Gamma mmax(j) := -\frac{D}{\Delta r}\cdot\left(N_{j,mmax} - N_{j,mmax-1}\right)$$

This is the loss flux at the left side of the cell (mmax-1, mmax).

$$Loss := \sum_{j=0}^{jmax-1} \left[2\cdot\pi\cdot(mmax\cdot\Delta r)\cdot(\Gamma mmax(j)\cdot\Delta t)\right]$$

This is the sum of the losses at the right boundary. The loss per unit time per unit circumference Γ has been multiplied by $2\ \pi\ r\ \Delta r\ \Delta t$.

$Loss = 33.221$

$$Initial := \sum_{m=0}^{mmax} \left(2\cdot\pi\cdot r_m\cdot N_{0,m}\cdot\Delta r\right) \qquad Initial = 33.822$$

The initial number of particles is found by summing the particles in each cell at the time step j = 0. Recall that each cell is a ring with area $2\pi r\Delta r$.

$$Final := \sum_{m=0}^{mmax} \left(2\cdot\pi\cdot r_m\cdot N_{jmax,m}\cdot\Delta r\right) \qquad Final = 0.601$$

The final number of particles is found by summing the particles in each cell at the time step j = jmax.

$$Gain := S\cdot\pi\cdot(mmax\cdot\Delta r)^2\cdot(jmax\cdot\Delta t) \qquad Gain = 0$$

This is the number of particles added to the left of the last cell.

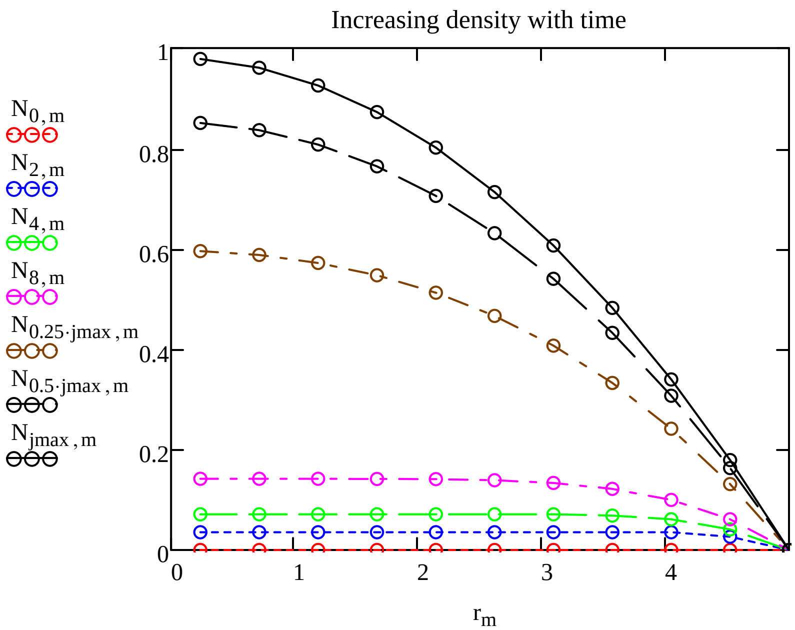
Note that the change in the number of particles, (Final-Initial), is very near to the gain in particles minus the loss of particles (Gain-Loss).

$(Final - Initial) - (Gain - Loss) = -1.985 \times 10^{-4}$ Particle number is conserved vey well.

Cylindrical diffusion with a source term:

The number of particles created between the axis and r is S π r^2 per unit time. The diffusive flux $-2\pi rD$ (dn/dr) must remove these particles, so dn/dr = -Sr/2D and the number density must be n(x) = N [$1-(r/R)^2$] with N = SR^2 /4D. For a number density of 1.0, we need a source rate of $4D/R^2$. Now we will repeat the above example with the value of S that gives a density of 1.0 after a steady state is reached. We will use a starting density that is zero everywhere:

$g_m := 0$ $\quad S := \frac{4 \cdot D}{R^2}$ Find the new solution: $N := M(g, S)$



For this graph, the density begins at zero and increases in time.

$N_{jmax,0} = 0.978$ This is the final density nearest the origin.

Try it: Increase the maximum time tmax by a factor of 4, so that it is: Does the density approach unity at the center of the graph?

$tmax := \frac{8}{D}\left(\frac{R}{2.405}\right)^2$

Demonstration of particle conservation with a source term:

$$\Gamma mmax(j) := -\frac{D}{\Delta r}\cdot\left(N_{j,mmax} - N_{j,mmax-1}\right)$$

This is the loss flux at the left side of the cell (mmax-1, mmax).

$$Loss := \sum_{j=0}^{jmax-1} \left[2\cdot\pi\cdot(mmax\cdot\Delta r)\cdot(\Gamma mmax(j)\cdot\Delta t)\right]$$

$$Loss = 158.635$$

This is the sum of the losses at the right boundary. The loss per unit time is multiplied by Δt.

$$Initial := \sum_{m=0}^{mmax} \left(2\cdot\pi\cdot r_m\cdot N_{0,m}\cdot\Delta r\right) \qquad Initial = 0$$

The initial number of particles is found by summing the particles in each cell at the time step j = 0.

$$Final := \sum_{m=0}^{mmax} \left(2\cdot\pi\cdot r_m\cdot N_{jmax,m}\cdot\Delta r\right) \qquad Final = 38.426$$

The final number of particles is found by summing the particles in each cell at the time step j = jmax.

$$Gain := S\cdot\pi\cdot(mmax\cdot\Delta r)^2\cdot(jmax\cdot\Delta t) \qquad Gain = 197.061$$

This is the number of particles added to the left of the last cell.

$$Final - Initial = 38.426$$

$$Gain - Loss = 38.426$$

Note that the change in the number of particles, (Final-Initial), is very near to the gain in particles minus the loss of particles (Gain-Loss).

$$(Final - Initial) - (Gain - Loss) = -9.948\times 10^{-14}$$

Particle number is conserved vey well.

Reference:
The standard reference for solutions to the diffusion equation is *Conduction of Heat in Solids* by H. S. Carslaw and J. C. Jaeger (Clarendon Press, Oxford, 1959).