Computing Coursework: Simulating & evaluating the performance of an Aromatic Diffuser

A) What physics is this coursework trying to model and analyse?

The aim of this project is to develop a model for the diffusion of an aromatic diffuser placed at a position (x*,y*,z*)=(1.5, 2, 2) in a 5mx5mx5m room. The quantity of interest is ϕ, the density of the diffuser mixture (g/cm^3) in the room space over time modelled i.e. ϕ = ϕ(x,y,z,t) using the diffusion equation based upon the conservation of mass. The diffuser is modelled as a 4cmx4cmx4cm container with 75g of diffuser mixture that vapourises and diffuses out of the bottle over time (this is not a source, as the mass reduces over time).

A 3-dimensional space model is used over time (instead of 2D) despite the greater computation as it is more representative of the diffusion.

Figure 1: *A diffuser*
https://suppliesforcandles.co.uk/product/augeo-reed-diffuser-base

B) This model involves solving the 3D diffusion Partial Differential Equation (PDE) numerically:

$$\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}+\frac{\partial^2\varphi}{\partial z^2}=\frac{1}{D}\frac{\partial\varphi}{\partial t}$$

This is a parabollic PDE

D is the diffusivity of the diffuser in air 10^6 m^2 s^1. This is an estimation – *more information can be found in section G*.

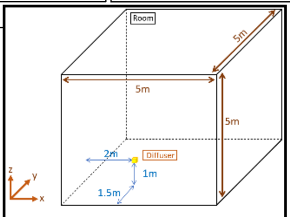


Figure 2: *Diffuser in room model*

C) Boundary value and initial values for my specific problem:

Boundary Conditions

$$\left.\frac{\partial\varphi}{\partial x}\right|_{x=0}=0 \qquad \left.\frac{\partial\varphi}{\partial y}\right|_{y=0}=0 \qquad \left.\frac{\partial\varphi}{\partial z}\right|_{z=0}=0$$

Perfume molecules cannot diffuse through the boundary wall (flux is 0)

$$\left.\frac{\partial\varphi}{\partial x}\right|_{x=L}=0 \qquad \left.\frac{\partial\varphi}{\partial y}\right|_{y=H}=0 \qquad \left.\frac{\partial\varphi}{\partial z}\right|_{z=Z}=0$$

L, H and Z are the dimensions of the room *(same reason as above)*

Initial Condition

$\varphi(x,y,z,0)=0$ $\qquad$ $\varphi(x^*,y^*,z^*,0)$ = density of diffuser = mass/volume = 75/(4*4*4) = 1.1719 g/cm^3

D) What numerical method I am deploying and why?

A numerical expression is obtained using the implicit Crank-Nicholson method instead of the explicit method, otherwise too high of a ratio between the space and time intervals to make the method convergent (r needs to be less than ½).
The solution to the implicit expression is found using the iterative Gauss Seidel Method (preferred over Jacobi, as Jacobi by definition requires the values to be stored and convergence is slower), which computes the solution without carrying out matrix operations (multiplications or inverses).
Solution using matrix inversion (Gauss elimination or algorithm in numpy library) is inefficient and requiring more steps, as a set of iterations is first required to inverse the matrix and then another set to find the solutions by matrix operations.

E) The discretisation used for the simulation is derived below (steps from continuous to discrete equation & boundary/initial conditions):

Starting from the mass diffusion PDE equation:

$$\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}+\frac{\partial^2\varphi}{\partial z^2}=\frac{1}{\alpha}\frac{\partial\varphi}{\partial t}$$

where $\varphi=\varphi(x,y,z,t)$ *and* φ *is density of diffuser mixture*

Forward difference in time and Central difference in space is applied (space intervals are dx, dy,dz;time intervals is k):

$$\frac{\varphi(x+dx,y,z,t)-2\varphi(x,y,z,t)+\varphi(x-dx,y,z,t)}{(dx)^2}+\frac{\varphi(x,y+dy,z,t)-2\varphi(x,y,z,t)+\varphi(x,y-dy,z,t)}{(dy)^2}+\frac{\varphi(x,y,z+dz,t)-2\varphi(x,y,z,t)+\varphi(x,y,z-dz,t)}{(dz)^2}=\frac{1}{D}\frac{\varphi(x,y,z,t+k)-\varphi(x,y,z,t)}{k}$$

Upon applying Crank-Nicholson method:

$$\frac{\varphi(x+dx,y,z,t+k)-2\varphi(x,y,z,t+k)+\varphi(x+dx,y,z,t)-2\varphi(x,y,z,t)+\varphi(x-dx,y,z,t)}{2(dx)^2}+\frac{\varphi(x,y+dy,z,t+k)-2\varphi(x,y,z,t+k)+\varphi(x,y+dy,z,t)-2\varphi(x,y,z,t)+\varphi(x,y-dy,z,t)}{2(dy)^2}+$$
$$\frac{\varphi(x,y+dy,z,t+k)-2\varphi(x,y,z,t+k)+\varphi(x,y+dy,z,t)-2\varphi(x,y,z,t)+\varphi(x,y-dy,z,t)}{2(dz)^2}=\frac{1}{D}\frac{\varphi(x,y,z,t+k)-\varphi(x,y,z,t)}{k}$$

Setting uniform space intervals $dx=dy=dz=h$ and $r=\frac{k}{h^2}$, and the equation is simplified to:

$$\left(\frac{2}{D}+6r\right)\varphi_{x,y,z,t+k}=\left(\frac{2}{D}-6r\right)\varphi_{x,y,z,t}+r\left(\varphi_{x+h,y,z,t}+\varphi_{x-h,y,z,t}+\varphi_{x,y+h,z,t}+\varphi_{x,y-h,z,t}+\varphi_{x,y,z+h,t}+\varphi_{x,y,z-h,t}+\varphi_{x+h,y,z,t+k}+\right.$$
$$\left.\varphi_{x-h,y,z,t+k}+\varphi_{x,y+h,z,t+k}+\varphi_{x,y-h,z,t+k}+\varphi_{x,y,z+h,t+k}+\varphi_{x,y,z-h,t+k}\right)$$

Conclusively, the following simplified expressions is solved with Gauss-Seidel iterations in the code:

$$\varphi_{x,y,z,t+k} = \frac{\left(\frac{2}{D} - 6r\right)\varphi_{x,y,z,t} + r\left(\varphi_{x+h,y,z,t} + \varphi_{x-h,y,z,t} + \varphi_{x,y+h,z,t} + \varphi_{x,y-h,z,t} + \varphi_{x,y,z+h,t} + \varphi_{x,y,z-h,t} + \varphi_{x+h,y,z,t+k} + \varphi_{x-h,y,z,t+k} + \varphi_{x,y+h,z,t+k} + \varphi_{x,y-h,z,t+k} + \varphi_{x,y,z+h,t+k} + \varphi_{x,y,z-h,t+k}\right)}{\left(\frac{2}{D} + 6r\right)}$$

<u>Initial Condition *(is already discretised)*</u>

$\varphi(x, y, z, 0) = 0,\ \varphi(x^*, y^*, z^*, 0)$ = density of diffuser = mass/volume *where x*, y*, z* is the position of the diffuser*

<u>Boundary Conditions using Euler methods</u>

By forward Euler:

$$\left.\frac{\partial\varphi}{\partial x}\right|_{x=0} = \frac{\varphi_{(x_0,y,z,t)} - \varphi_{(x_1,y,z,t)}}{h} = 0$$

$\therefore\ \varphi_{(x_0,y,z,t)} = \varphi_{(x_1,y,z,t)}$ And similarly for y&z: $\varphi_{(x,y_0,z,t)} = \varphi_{(x,y_1,z,t)}$, $\varphi_{(x,y,z_0,t)} = \varphi_{(x,y,z_1,t)}$

By backward Euler:

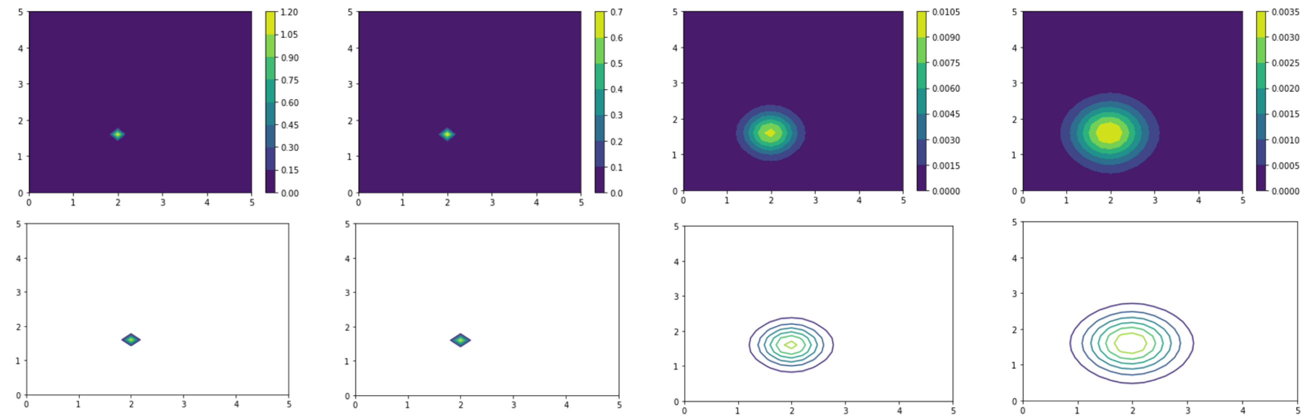
$$\left.\frac{\partial\varphi}{\partial x}\right|_{x=L} = \frac{\varphi_{(x_N,y,z,t)} - \varphi_{(x_{N-1},y,z,t)}}{h} = 0$$

$\therefore\ \varphi_{(x_N,y,z,t)} = \varphi_{(x_{N-1},y,z,t)}$ And similarly for y&z: $\varphi_{(x,y_N,z,t)} = \varphi_{(x,y_{N-1},z,t)}$, $\varphi_{(x,y,z_N,t)} = \varphi_{(x,y,z_{N-1},t)}$

F) Plots of the numerical results comprehensively and discussions can be found below. The model was run for a period of up to 30 days and insights and evaluations on the performance of an aromatic diffuser are shown below.

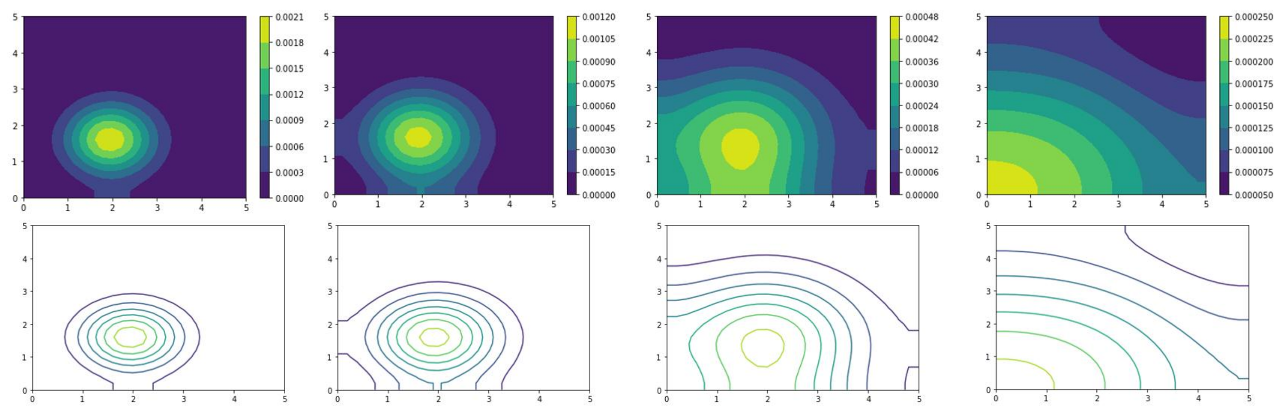
Plots of in the xy-plane where the diffuser is located is shown over time in figures 3 and 4 below.

Diffusions seems initially slow, as there seems to be a high concentration remaining at the diffuser for almost a day after which it begins to visibly distribute more evenly to the rest of the room. During the diffusion process, there are circular contours suggesting diffusion is occurring evenly in all directions around the diffuser, as expected. As the mixture spreads, the density around the location of the diffuser decreases, and the overall density values throughout the space are getting closer to each other (field is becoming more uniform).



t = 1 min t = 1 hour t = 1 day t = 2 days

Figure 3: *Coloured Contour Plots of diffuser mixture density in xy-plane of the room over 2 days*



t = 3 days t = 5 days t = 10 days t = 30 days

Figure 4: *Coloured Contour Plots of diffuser mixture density in xy-plane over 30 days*

It has been shown that a 75ml and 10^{-6} diffusivity diffuser lasts for almost 30 days before it reaches undetectable values ($<0.0001 g/cm^3$), which matches the common manufacturers' claims on websites that the fragrance can last up to a month.

F) Results (Continuation)

Whilst it would have been expected that there is a uniform distribution on the diagram after 30 days, there seems to be some variation. The values nevertheless are so small throughout the whole area and lower than the tolerance for the iterations set by the code (0.001), and suggesting that the disparity to be due to error in the numerical method (decreasing tolerance even further results in a larger number of iterations than the computer can handle).

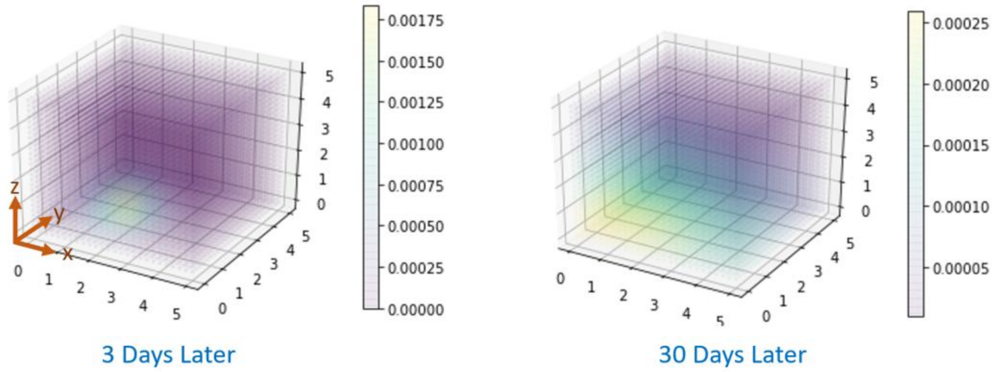


Figure 5: *3D plots (x,y,z) of Coloured Contour Plots of diffuser mixture density in x-y plane over 30 days*

Additionally, using the solution outputted over time, the mass of fluid left in the diffuser (calculated by mass = ϕ x Volume where ϕ is the density at the location of the diffuser) over time is plotted in figure 6 below.

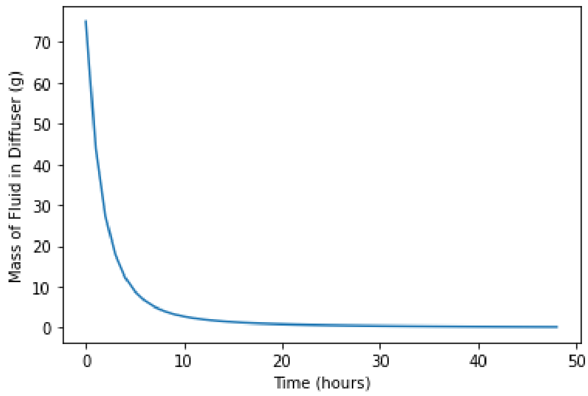


Figure 6: *Mass of diffuser mixture left in the container over time*

The graph shows that after 20 hours (~1 day), the diffuser has become nearly empty with an insignificant amount of fluid left in the container, suggesting that the air in the room has reached close to saturation after this point in time.

<u>Testing code at 10 and 50 times finer intervals (dx, dy, dz and dt have been divided by 10 and 50):</u>

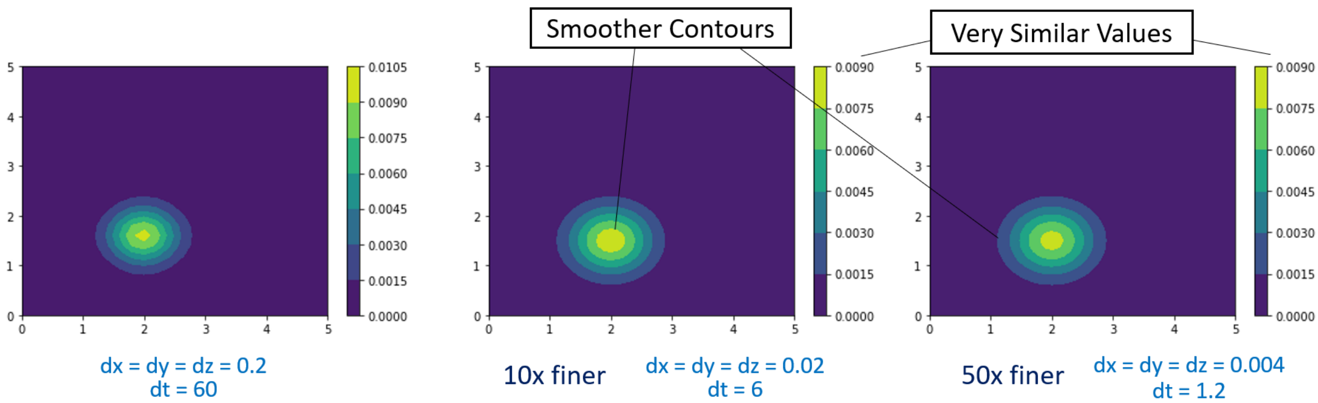


Figure 7: *Mass of diffuser mixture left in the container over time*

On choosing a 10 times finer grid, the values seem smaller and contours are smoother, implying there is a considerable accuracy lost at the grid size used for the results. However, the difference between the 10 and 50 times finer grids is minimal. This suggests there is convergence, as expected by the implicit nature of Crank-Nicholson.

G) Other remarks (limits of the model, convergence problems, possible alternative approaches, anything you find relevant and important to mention):

The model assumes no obstructions in the room apart from the walls. Obstructions could not be generally modelled as these (humans and objects blocking the diffusion of the odour) vary on a room-by-room basis. Obstructions can be accounted by defining a new geometry of the room (i.e. grid is not cubic but an irregular mesh).

No leakage of air is also assumed in the model, which is not realistic if there is door or a window that is opened.

It should be mentioned that the value of diffusivity used in this model is an average of the values obtained from the paper *The diffusion of perfume mixtures and the odor performance on diffusivity constants of commercial perfume*, Miguel A. Teixeira (2009). However, if the diffusivity of a mixture of known consistency is to be determined, the following equation modified by Fuller may be used:

$$D_{AB} = \frac{0.00143 \times T^{1.75}}{P \times {M_{AB}}^{\frac{1}{2}} \left[(\Sigma_v)_A^{\frac{1}{3}} + (\Sigma_v)_B^{\frac{1}{3}} \right]^2}$$

where D_{AB} is the diffusivity constant of a gas A diffusing in a gas B, T is temperature, P is pressure, Σ_v is the atomic diffusion volume of each substance, and M_{AB} is defined as:

$$M_{AB} = 2 \times \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{-1}$$

Where M_A and M_B are the molecular weights of the two substances. Typically, gas B is air, and gas A the perfume mixture.