BENG 221 Problem Presentation Report

Introduction

Consider this analogy of diffusion of particles in a macroscopic world without convection. A certain man is late to a restaurant for a date. He becomes nervous and starts sweating, producing body odor. To mask this odor, he applies cologne. In this situation, please consider the following:

1. Determine D_{Odor} using the following statement: "Without convection, it would take a year to smell one's own feet." The temperature is 293 K. Assume the body odor particles emitted by the feet are the same as the ones emitted by the man.
2. Determine the initial concentration C_0 also using the above statement. Assume that detection occurs at 0.1 mol/m^3 and the distance between nose and feet is 5 feet. You can treat the dimension from nose to feet as semi-infinite.
3. If he sits roughly 0.1 m away from his date at the restaurant, which would his date smell first, the cologne or the body odor? The diffusion constant of the perfume, $D_{Perfume}$ is 1.25 x 10^{-5} m^2/s.[1] Use Matlab's *pdepe* solver to numerically approximate your answers where L = 2 m. At what time does the person detect the perfume? The odor?
4. Calculate the size of the odor particle using experimental formulation for the diffusion constant at 293 K.
5. What would happen to the solution for odor if the temperature was increased by 10 K? 20 K? Decreased by 10 K? Plot each solution using *pdepe*.
6. What would happen to the solution for odor if the humidity was 25%? 50%? 75%? Plot each solution using *pdepe*.
7. What would happen if the particle size of the odor was 3 pm? 3 fm? 3 am? Plot each solution using *pdepe*.
8. Now assume convection does occur by inserting a positive source term in your numerical approximation. Estimate the value of the source term such that the body odor is detected around the same time as the cologne.

This problem will show that diffusion is not the only way particles move in the macroscopic world, and that convection is the primary reason why particles such as smells in the air move so fast. Without convection, particles would move very slowly, which is indicative in the very long odor/perfume detection times for which the student will solve. However, diffusion is very important in the microscopic world, such as in cells, since the distances over which particles diffuse is in the nanometer scale. In the macroscopic world, convection dominates over diffusion. A practical application of our problem is in detecting leakage of poisonous/flammable gases. For example, Liquefied Petroleum Gas (LPG) is an odorless natural gas which is used in gas stoves. It is highly flammable and thus any leakage needs to be immediately detected. This is done by mixing LPG with hydrogen sulfide, which on leaking diffuses 10^5 times faster than LPG creating a pungent smell indicating the presence of a leak.

This problem is also important because it bridges the ideas of diffusion and Brownian motion (in fact they may be two different ways of looking at the same thing) and also shows that the diffusion constant is not a constant at all and can vary with temperature, viscosity, particle size, etc.

Set-up

1. Determine D_{Odor}

[1] Teixeira, M et al, "The diffusion of perfume mixtures and the odor performance", *Chemical Engineering Science*, Volume 64, Issue 11, 1 June 2009, Pages 2570-2589

Use Brownian motion, which is the motion of particles suspended in viscous fluid resulting from fluctuating forces due to collisions with other molecules. It is a stochastic process with continuous paths and stationary, independent increments.

Use the 1D equation of motion to obtain an expression to solve for D_{Odor} using the above statement.

$$X - f\dot{x} = m\ddot{x}$$

where

$$\begin{aligned} X &= \text{ random force from collision} \\ f &= 6\pi n R = \text{ friction coefficient} \\ \eta &= \text{ viscosity} \\ R &= \text{ radius of particle} \end{aligned}$$

2. Determine C_0

Use Fick's 2nd law of diffusion assuming semi-infinite x-dimension:

$$\frac{\partial C}{\partial t} = D_{\text{Odor}} \frac{\partial^2 C}{\partial x^2}$$

$$\begin{aligned} &\text{IC: } C(x,0) = 0 \\ &\text{BC: } C(0,t) = C_0 \\ &\text{BC: } C(\infty,t) = 0 \end{aligned}$$

The initial condition states that before t = 0 there is no odor. The first boundary condition assumes that at the feet, the concentration is always C_0. At infinity, there is also no odor.

4. Calculate the size of the odor particle

The experimentally found formula for diffusion constant is:

$$D = \frac{kT}{f}$$

where

$$\begin{aligned} k &= \text{Boltzmann Constant} \\ T &= \text{temperature} \\ f &= \text{Friction coefficient} \end{aligned}$$

Assumptions

1. There is no convection, particles move by diffusion only
    a. This assumption is unrealistic but valid because otherwise the process would be dominated by convection
2. Body odor particles are the same as odor particles from feet
    a. Although the two particles may be different, the assumption is reasonable because it is likely that they are not different in size or diffusion constant.
3. Detection of an odor occurs at 0.1 mol/m^3
    a. This is reasonable because everyone has a natural body odor that we cannot detect on a normal basis. We can only smell odor when its particularly strong, and hence the assumption that concentration needs to exceed 0.1 mol/m^3 for detection is acceptable.
4. The diffusion constants do not vary within a solution, but may vary between solutions.
    a. This is not reasonable because the diffusion constant may vary in real-life at any time.

5. In Part 3, body odor is radiated from the whole body uniformly
    a. This is not reasonable because there are probably certain areas such as feet or underarms that are more odorous than others.

Solution

1. Determine D_{Odor} (analytical derivation found in Lecture 14)

$$D = \frac{x_{rms}^2}{2t} = \frac{(1.524\text{ m})^2}{2(31536000\text{ s})} = 3.69 \text{ x } 10^{-8}\text{ m}^2/\text{s}$$

where t is time.

2. Determine C_0 (analytical derivation in **Appendix A**)

$$C_0 = C\frac{1}{\operatorname{erfc}\left(\frac{x}{2}\sqrt{\frac{1}{Dt}}\right)} = 0.3152\text{ mol/m}^3$$

3. Is the odor or cologne detected first? When is each odor detected? (Using pdepe)

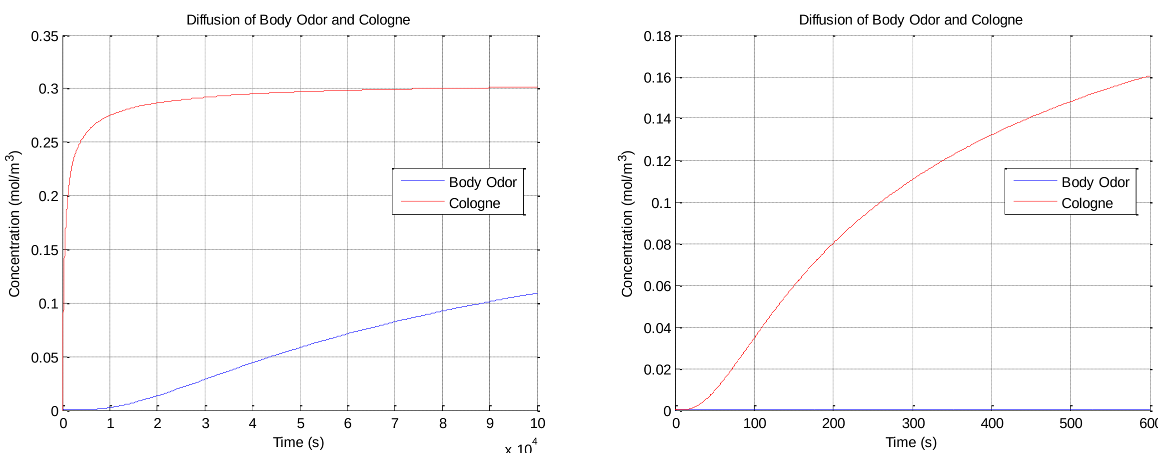


Figure 1. Body Odor and Cologne (left graph goes to 10^5 s)

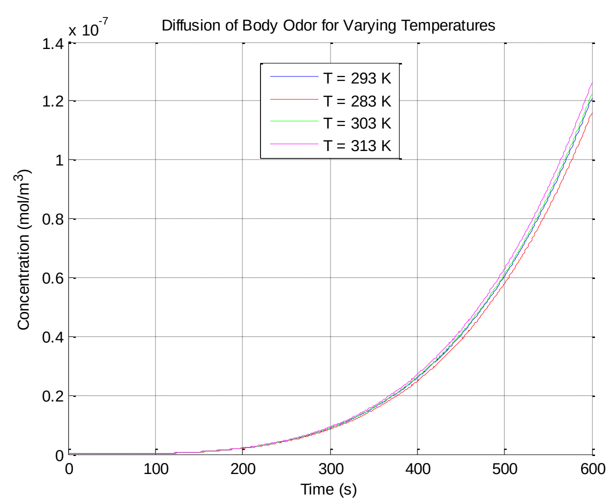
Using the analytical solution and diffusion constant calculated above, the concentration of body odor with time at a distance of 0.1m can be plotted as shown in **Figure 1**. The odor takes 88640 s or approximately 24 hours to be detected at a concentration greater than 0.1 mol/m^3 across the table (0.1 m) in comparison to the cologne which takes 261.5 s or about 4 min.

4. Calculate the size of the odor particle

$$D = \frac{kT}{f} = \frac{RT}{N}\frac{1}{6\pi\mu r} \Rightarrow r = \frac{RT}{N}\frac{1}{6\pi\mu D}$$
$$= 3.0848 \text{ x } 10^{-10}\text{ m}$$

5. Varying Temperature

Varying the temperature of the room affects the diffusion constant. The increasing temperature also affects the viscosity of the air. As seen in **Figure 2**, the rate of diffusion increases with increase in



temperature due to the increase in thermal motion of the odor particles. This is in accordance to the relation that the diffusion constant is proportional to temperature.

6. Varying Humidity

As the humidity in the air increases, the viscosity of the air decreases. Since diffusion in inversely proportional to viscosity, as expected in **Figure 3**, the diffusion is slowest at 1% humidity and increases with increasing water vapour concentration.

7. Varying Particle Size

Diffusion also depends on particle size. As seen in figure, as the particle size increases the diffusion rate decreases, which is in accordance to the relation that the diffusion constant is inversely proportional to particle radius. An increase in particle size would result in a heavier molecular and thus, a slower rate of diffusion. The femtometer scale particles diffuse exponentially compared to the picometer particles. This is evident in the body odor which consists of particles in the range of picometer to nanometer when compared to the faster diffusing perfume composed of femtometer particles. At the attometer level, the diffusion is almost instantaneous. Thus , the smaller the particle radius, the more effective the perfume.

8. With Convection

Using a source term of roughly 0.05 mol/(s·m^3), the time of detection decreases to about 250 s. This is a more reasonable time of detection for a person sitting about 0.1 m away, depending how strong the initial concentration is. However, this result is slightly unrealistic because the source term inherently "creates" more particles, where as convection is simply supposed to move them faster.

Conclusions

Thus, based on the above solutions, we can conclude that the man's date will be safe from his body odor. The impact of varying temperature and viscosity is not significant because the diffusion constant of the odor is very small to begin with, provided the variations are not extreme. On the other hand, the size of the diffusing particle is very

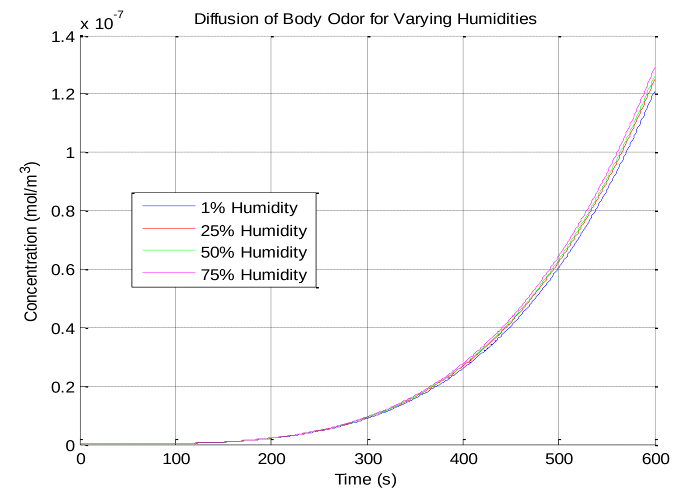


Figure 3. Varying Humidity

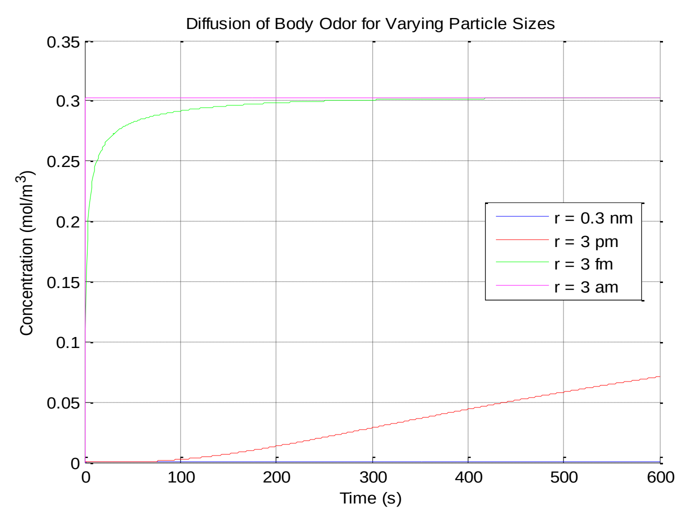


Figure 4. Varying Particle Size

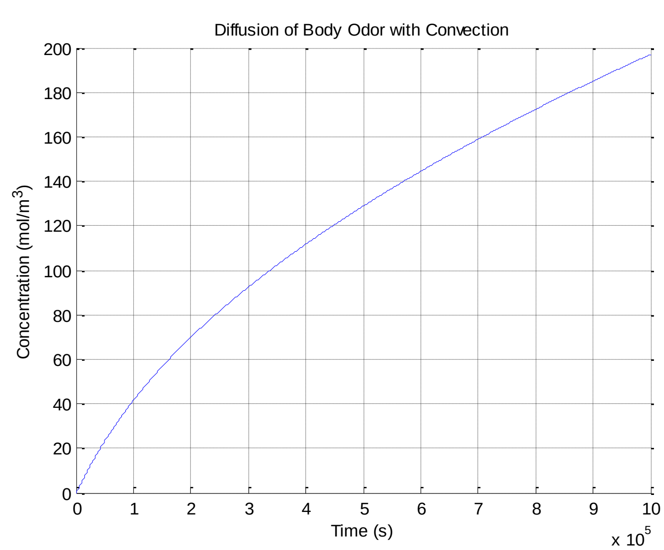


Figure 5. With Convection

important to ensure that the perfume will diffuse faster than the body odor.

Analogous to the microscopic scale, such as calcium diffusion in cardiomyocytes, these factors have a much more significant role to play since diffusion occurs over distances on the order of nanometers. In choosing indicator gases for poisonous substances, it is useful to take into consideration the particle size since a smaller particle will diffuse faster. Also, one needs to run experiments/simulations to ensure that the indicator gas can diffuse effectively in varying temperature and humidity conditions.

Our analytical solution is based on the approximation that it takes a man a year to smell his own feet in the absence of convection. Eliminating convection from the problem explains why it takes over 1 day for the body odor to reach the date. This assumption is not realistic since at the macroscopic scale, convection is the dominant process. Also, the diffusion constant for the odor needs to be experimentally determined for the solution to be more realistic.

Future Work

In order to mimic convection for our question we altered the source term in the diffusion equation. Although this might produce reasonable results, adding a source term does not necessarily represent convection. Some reasons why include the fact that convection has a direction, convection is not a source and thus does not create new particles, and also convection is a separate process from diffusion and cannot in a technical sense be incorporated into a diffusion equation. Thus, in our future work, we will model the effects of convection alone due to the fact that convection is dominant and fast acting compared to the effects of diffusion. The concentration profile could be obtained for the steady-state situation, utilizing Fick's law. However, if we want a concentration profile which varies with time more techniques specific to mass transfer would be required. This may be possible but extends beyond the scope of this class.

Also, the cologne concentration should decrease with time, whereas in our model the person has a "fixed" concentration of cologne, invariant of time since we assume the initial concentration is so large compared to the amount diffusing away. In order to compensate for this we could make the boundary condition a function of time.

Appendix A.
Analytical derivation of solution

$$\frac{\partial C}{\partial t} = D_{\mathrm{Odor}} \frac{\partial^2 C}{\partial x^2}$$

$$\mathrm{IC}: C(x,0) = 0$$
$$\mathrm{BC}: C(0,t) = C_0$$
$$\mathrm{BC}: C(\infty,t) = 0$$

Laplace above with respect to time, hence t→s (in Laplace domain)

$$s(x,s) - C(x,0) = D\frac{d^2C}{dx^2}$$

Apply the initial condition:

$$\mathrm{IC}: C(x,0) = 0$$

Rearranging

$$\frac{d^2C}{dx^2} - \frac{s}{D}(x,s) = 0$$

The general solution to this is

$$C(x,s) = c_1 e^{r_1 x} + c_2 e^{r_2 x}$$

The characteristic equation and roots of the Laplace transformed differential equation are

$$r^2 - \frac{s}{D} = 0$$
$$r = \pm\sqrt{\frac{s}{D}}$$

Applying the boundary conditions (which must be Laplace transformed), solve for c_1 and c_2:

$\mathrm{BC1}: C(\infty,t) = 0$

$$0 = \ c_1 e^{+\infty} + c_2 e^{-\infty}$$
$$c_1 = 0$$

$\mathrm{BC2}: C(0,s) = \frac{C_0}{s}$

$$\frac{C_0}{s} = c_1 + c_2$$
$$\frac{C_0}{s} = c_2$$

Substitute in constants:

$$C(x,s) = \frac{C_0}{s} e^{-\sqrt{\frac{s}{D}}x}$$

Recall the Laplace transform of the erfc:

$$\mathcal{L}\left(erfc\left(\frac{a}{2\sqrt{t}}\right)\right) = \frac{e^{-a\sqrt{s}}}{s}$$

In our case

$$a = \sqrt{\frac{1}{D}} * x$$

Thus the inverse Laplace of $C(x, s)$ to get analytical solution:

$$C(x,t) = C_0 erfc\left(\sqrt{\frac{1}{Dt}} * \frac{x}{2}\right)$$

Appendix B. Matlab m-files (appended)