

Transport Phenomena:

I. From Brownian motion to mass transport equations

Take home message:

Fick law for mass:

$$\mathbf{J}_i = -D_i \nabla c_i$$

J_i mass or molar flux, c_i mass or molar concentration, D_i diffusion coefficient [m²/s].

Mass transport equation (for non compressible fluid and dilute solute):

$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c = \alpha \Delta c + r_i$$

D_i mass diffusion coefficient [m²/s], r_i source or sink of species i .

Lecture notes on: <https://blog.espci.fr/mecaflu/transport-phenomena/>

1 Syrup in a glass of water

Consider a glass containing a layer of colored syrup where water has been gently added to prevent mixing (Fig. 1). Does this apparently stable configuration correspond to a thermodynamic equilibrium?

In a very idealized description, sugar molecules could be considered as particles of radius $a \sim 1$ nm, of density $\rho_s = 1.6 \cdot 10^3$ kg/m³. What would be the vertical distribution of the concentration if we wait for equilibrium?

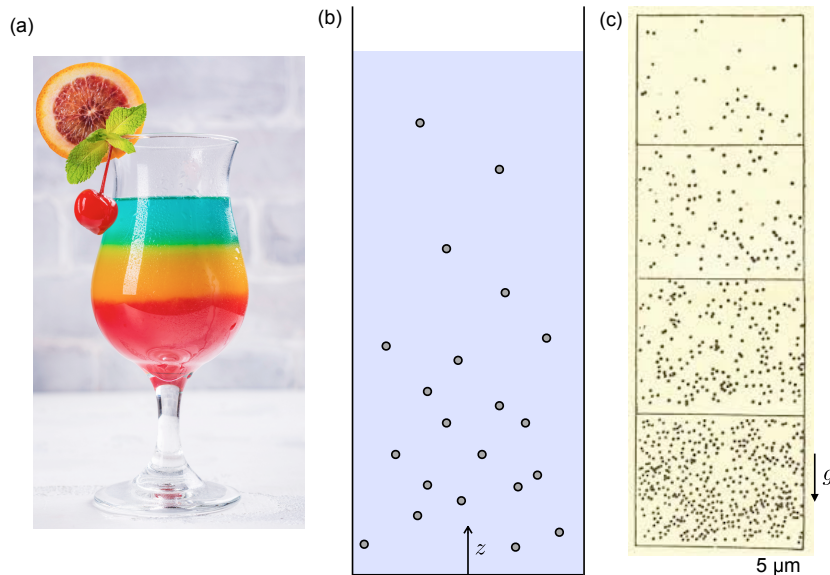


Figure 1: **a.** Layered cocktail: does it correspond to a thermodynamic equilibrium state? **b.** Idealized version sugar molecules viewed as a perfect gaz. **c.** Actual experiment from Jean Perrin conducted in 1909 with resin particles of 0.6 μm of diameter.

Did you know that monitoring the density of microparticles suspended in a solution led Jean Perrin to win the Nobel prize in 1926 for his estimation of Avagadro number? Here is the brilliant idea: the particles were small enough to undergo thermal motion but still large enough to be visible (with a microscope). At the time of his discovery (~ 1910) this was the ultimate proof of the atomistic nature of matter.

Diffusion can be viewed as a random walk. In a very simplified description, we consider that at every time step τ particles jump randomly over a distance ℓ in the x , y or z direction (Fig. 2). How does the mean square displacement evolves with time?

If the particles move at a typical velocity $U = \ell/\tau$, what is the viscous force the particles undergo? The corresponding energy is compensated by the thermal energy $k_B T$. What is the scaling for the diffusion coefficient? Provide an order of magnitude for sugar molecules. How long would we have to wait for the layers of the cocktail to vanish?

Using the same ideal model, we now consider a surface separating a region of particle concentration $c + \delta c$ from a region of concentration c . Derive the mass flux as the concentration tends to equilibrate.

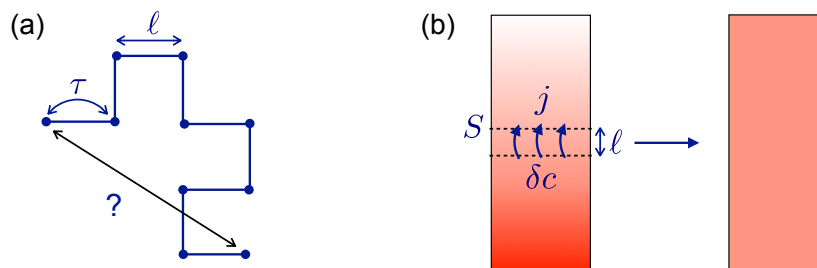


Figure 2: **a.** Random walk of a particle viewed as jumps of length ℓ at every time step τ . **b.** Particle flux through a surface during a time step τ .

2 Adding convection

Obviously, stirring the cocktail tends to homogenize the cocktail. Convection should thus be added to diffusion in the mixing process.

Consider an arbitrary volume of the space Ω or area S through which the liquid flows. What is the global flux resulting from convection across the surface of this elementary volume? What is the flux corresponding to diffusion? Derive the temporal evolution of the concentration inside the volume by simple mass conservation and using the divergence theorem. We will here assume that the concentration is very dilute so that convection only involves the solvent velocity.

In the case of incompressible flows, another mass conservation relation comes into play. Derive the classical expression for the mass transport equation.