



# Introduction to Quantitative Geology

Lecturer: Ann-Kathrin Maier

Week 3 – Part 1: Natural diffusion



# Last week

- We talked about comparing predictions to observations:
  - Linear regression
  - Linear correlation
  - Goodness-of-fit

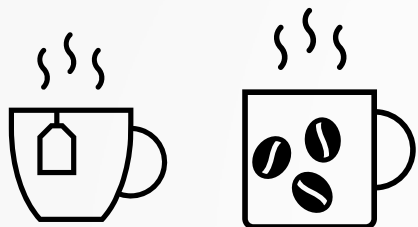


# This week

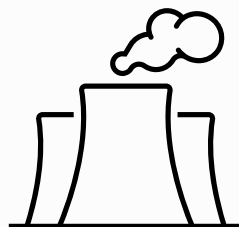
- **Part 1: Natural diffusion**
  - General concepts of diffusion
  - Mathematical definition
- **Part 2: Basic concepts of thermochronology**
  - What is it?
  - General terms and concepts



# Diffusion in daily life



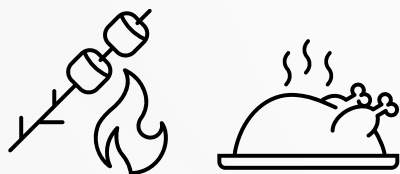
Brewing tea/coffee



Smoke in the air



Ink on paper



Heat in a solid (conduction)



CO<sub>2</sub> in a carbonated beverage



# Diffusion as a geological process: Landscapes



Moon surface (Eugene Cernan, 1972)

diffusion-dominated

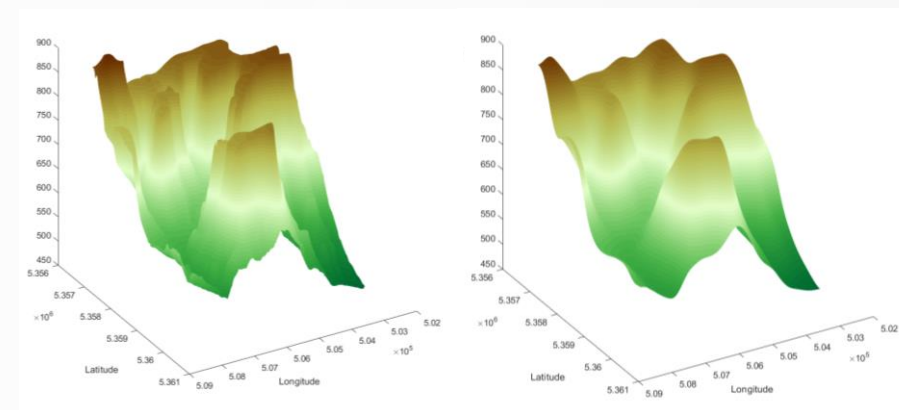


Tsingy de Bemaraha, Madagascar

dissolution-dominated



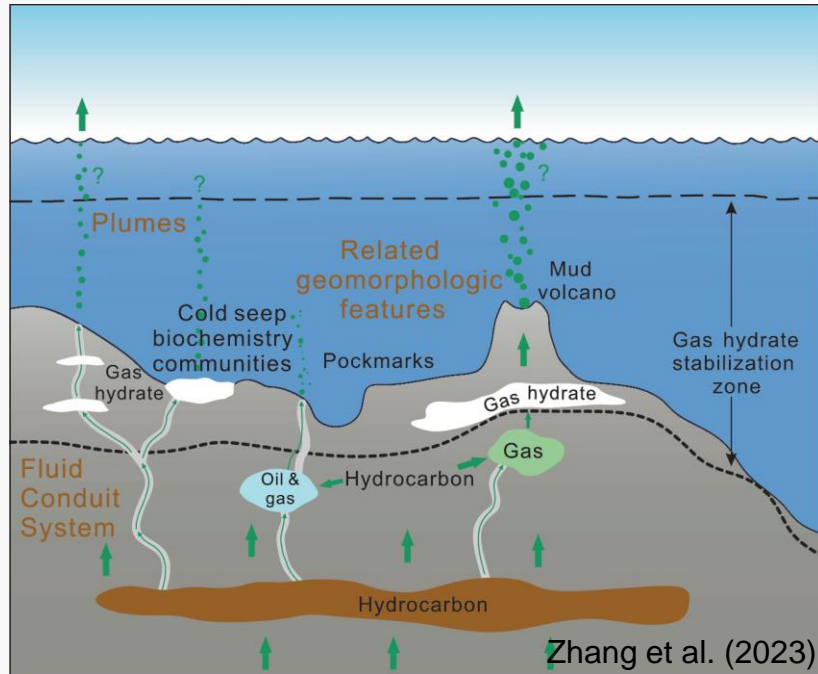
<https://commons.wikimedia.org/wiki/File:Moessingen-Rutschung-gross.jpg>



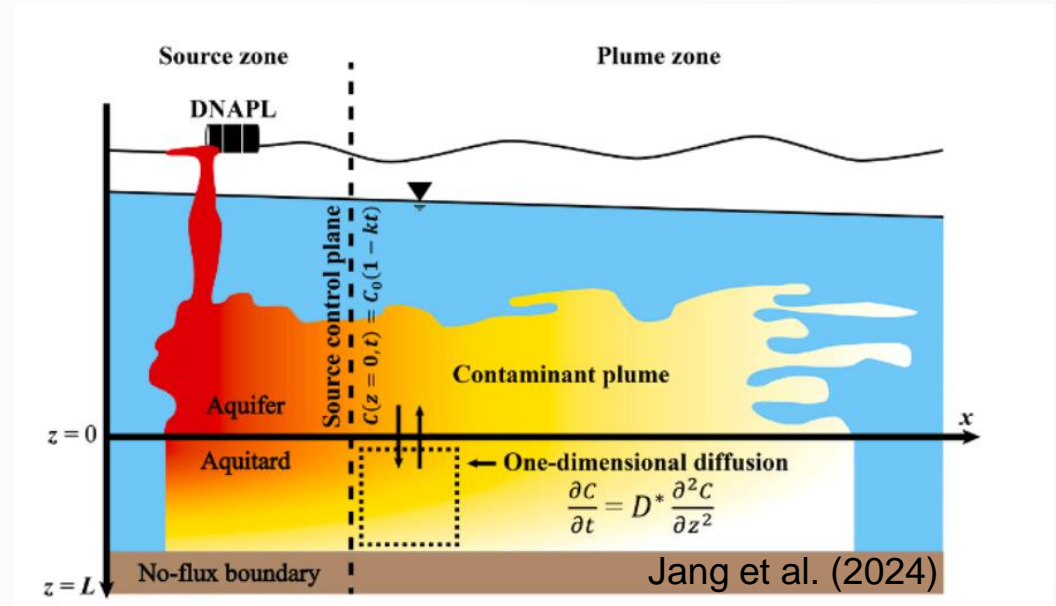
1 Myr of hillslope diffusion



# Diffusion as a geological process: Subsurface



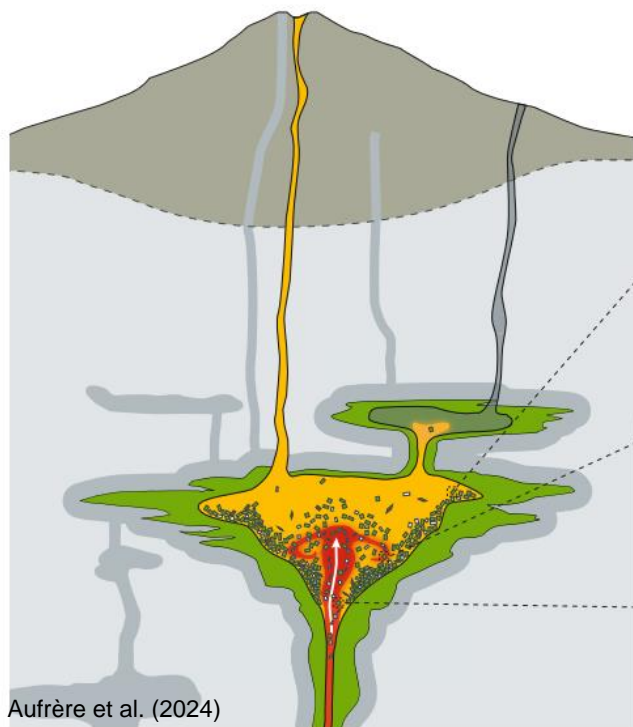
Gas seepage and migration



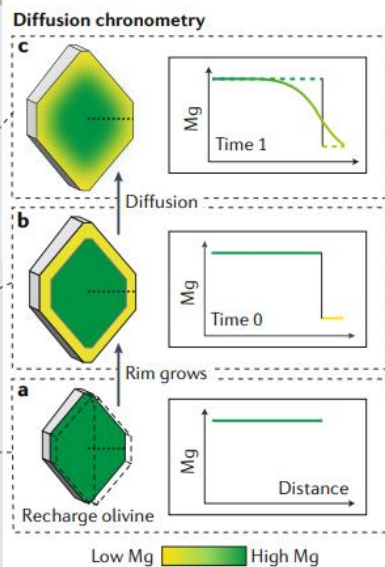
Pollutants in aquifers



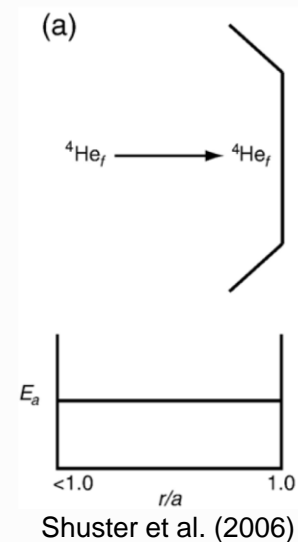
# Diffusion as a geological process: Mineral grains



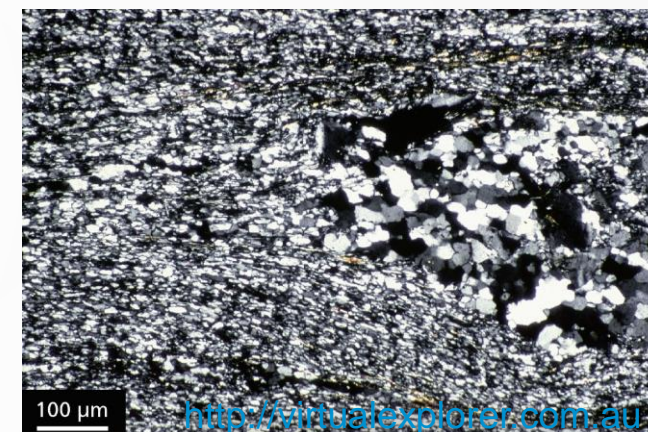
Aufrère et al. (2024)



Olivine diffusion chronometry



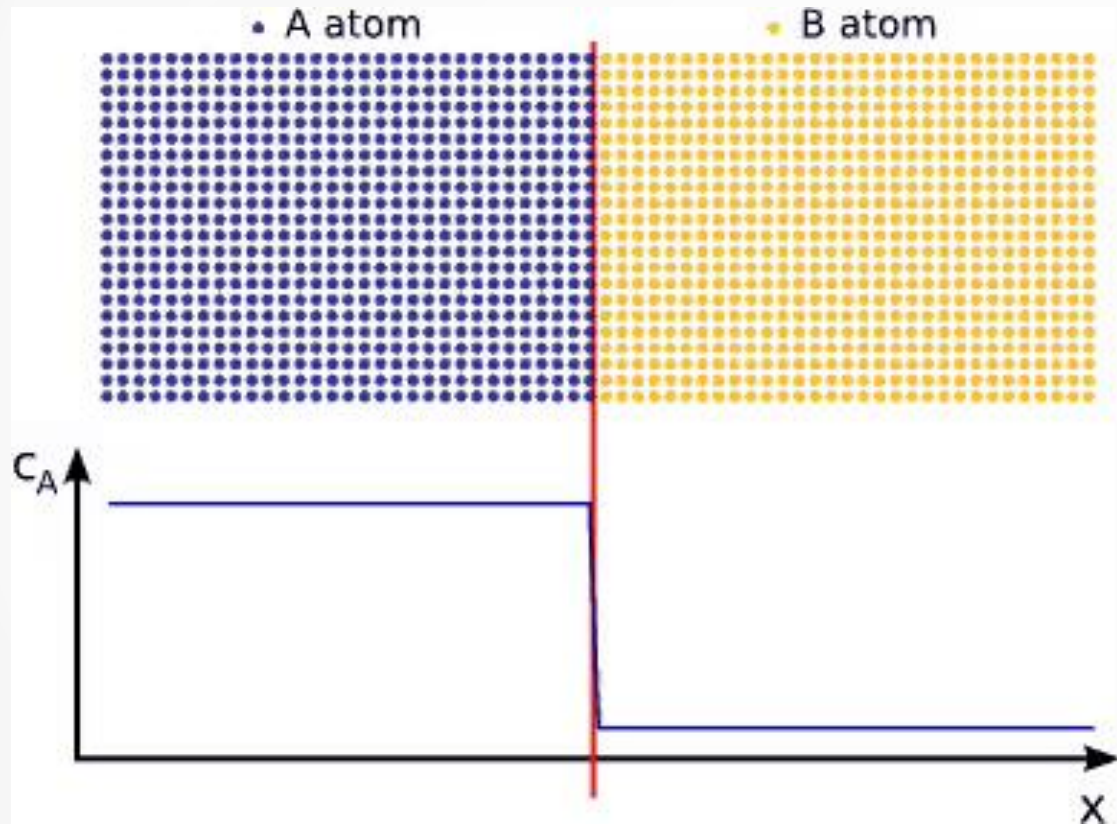
Diffusion of  ${}^4\text{He}$  in an apatite crystal



Grain boundary sliding



# The diffusion process



<http://web.unideb.hu/zerdelyi/>

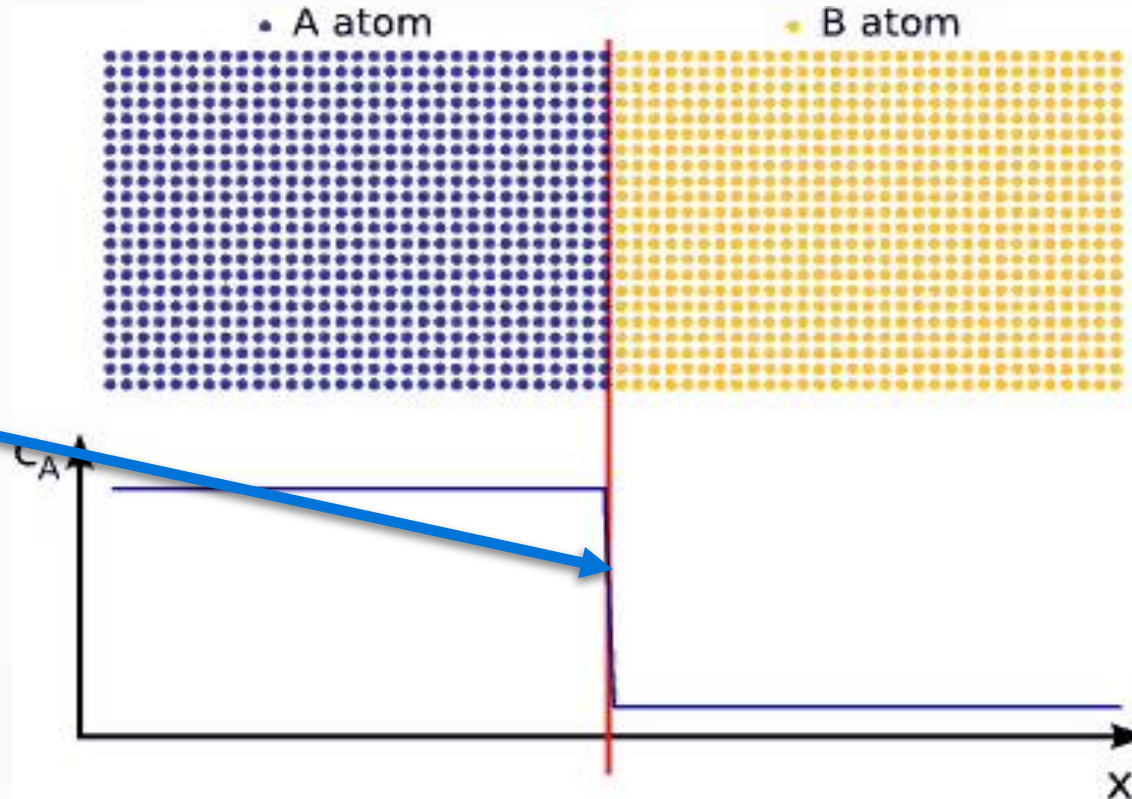
## Diffusion:

Process in which the random motion of particles results in mass transport or mixing



# The diffusion process

Concentration gradient



<http://web.unideb.hu/zerdelyi/>



# Describing diffusion

- Process in which the **random motion** of particles results in mass transport or mixing
- Net motion from regions of high concentration to regions of low concentration
- Leads to **reduction concentration gradients**



# Describing diffusion

- **Diffusion** occurs when a **conservative property** moves through space at a rate **proportional to a gradient**
- **Conservative property:** A quantity that must be conserved in the system (e.g., mass, energy, momentum)
- **Rate proportional to a gradient:** Movement occurs in direct relationship to the change in concentration



# Mathematical definition



# A mathematical definition

- **Diffusion** occurs when
  - 1) a **conservative property** moves through space
  - 2) at a rate **proportional to a gradient**
- From 2) :

[The transportation rate] is proportional to [the change in concentration over some distance]



# A mathematical definition

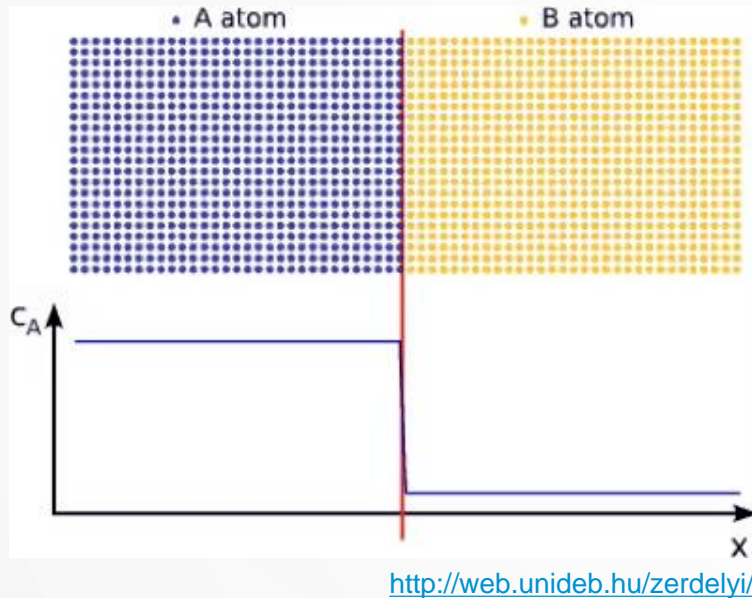
- In more quantitative terms: [The flux] is proportional to [the concentration gradient].
- As an equation:

$$q \propto \frac{\Delta C}{\Delta x}$$

where  $q$  is the (mass) flux,  $\propto$  is the “proportional to” symbol,  $\Delta$  indicates a change in the quantity that follows,  $C$  is the concentration and  $x$  is distance



# A mathematical definition

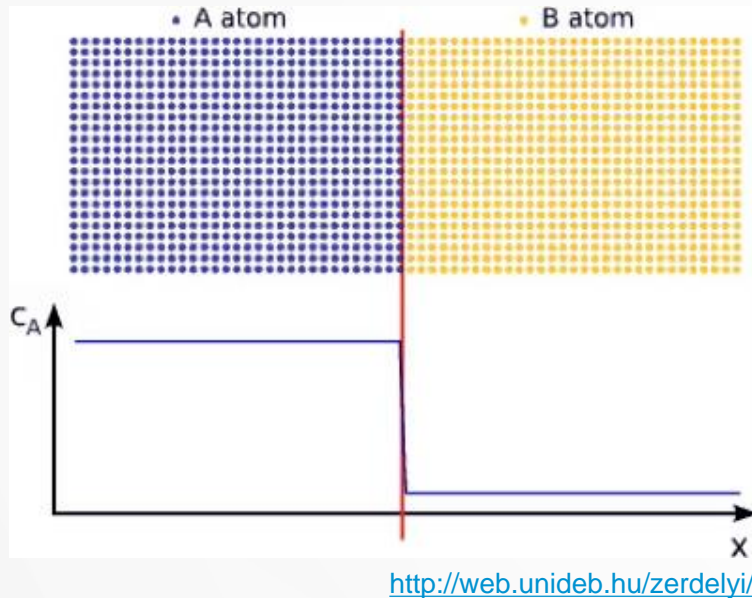


- If transport is directly proportional to the gradient, we can replace the proportional to symbol with a constant  $D$  (diffusion coefficient or diffusivity)
- We can also replace the finite changes  $\Delta$  with infinitesimal changes  $\partial$

$$q \propto \frac{\Delta C}{\Delta x} \quad \rightarrow \quad q = -D \frac{\delta C}{\delta x}$$



# A mathematical definition



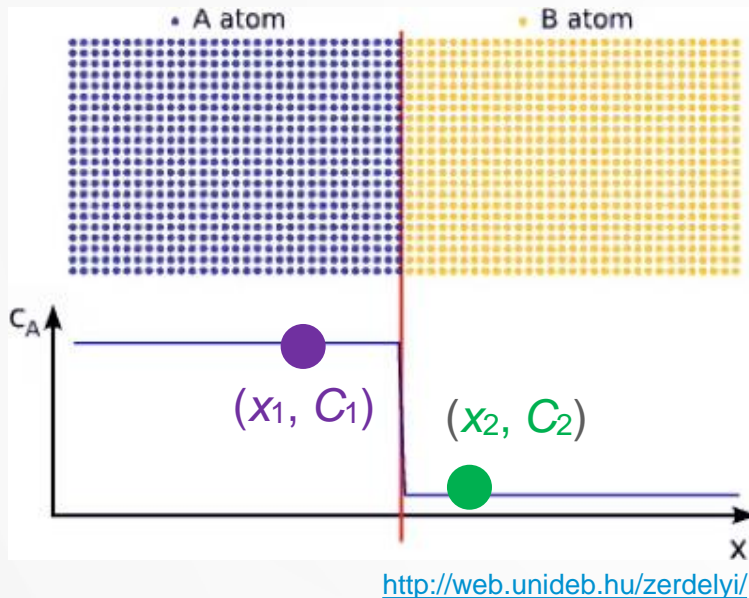
- Consider the example to the left:
- Here, we can formulate the diffusion of atoms of A across the red line with time as

$$q = -D \frac{\delta C_A}{\delta x}$$

where  $C_A$  is the concentration of atoms of A.



# A mathematical definition



- OK, but **why is there a minus sign?**
- We can consider a simple case for finite changes at two points:  $(x_1, C_1)$  and  $(x_2, C_2)$
- At those points, we could say

$$q = -D \frac{\Delta C}{\Delta x}$$

$$= -D \frac{C_2 - C_1}{x_2 - x_1}$$

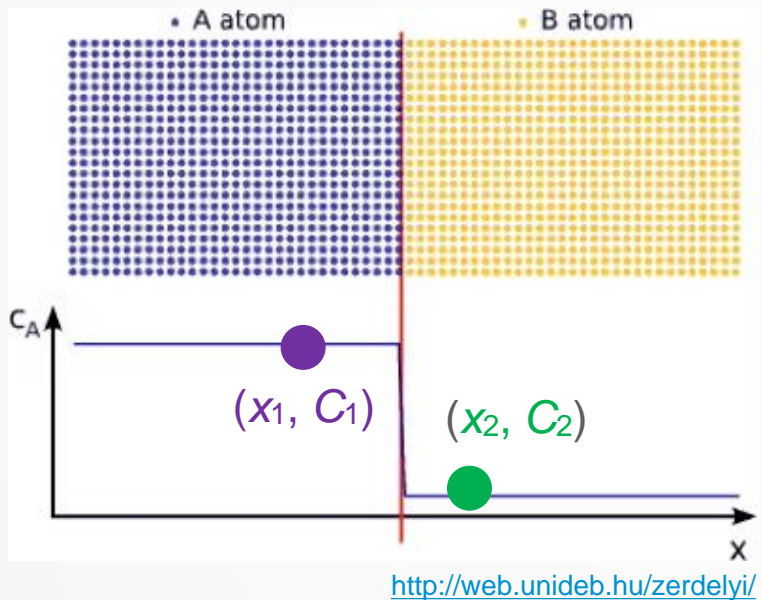
$\Delta C$  is negative  
 $\Delta x$  is positive

The gradient is negative!



# A mathematical definition

Positive flux of A



- Multiplying the negative gradient by  $-D$  yields a positive flux  $q$  along the  $x$  axis

$$q = -D \frac{\delta C_A}{\delta x}$$

$$q = -D \frac{\Delta C}{\Delta x}$$

$$= -D \frac{C_2 - C_1}{x_2 - x_1}$$



# A mathematical definition

- **Diffusion** occurs when
  - 1) a **conservative property** moves through space
  - 2) at a rate **proportional to a gradient**
- From 2) we got

$$q = -D \frac{\delta C_A}{\delta x}$$

where  $q$  is the (mass) flux,  $D$  is the diffusion coefficient,  $C$  is the concentration and  $x$  is distance



# A mathematical definition

- What about “ 1) a **conservative property moves through space**” ?

- We can say:

[change in concentration with time] is equal to [change in transport rate with distance]

- In slightly more quantitative terms:

[rate of change of concentration] is equal to [flux gradient]



# A mathematical definition

- [rate of change of concentration] is equal to [flux gradient]
- As an equation:

$$\frac{\Delta C}{\Delta t} = - \frac{\Delta q}{\Delta x} \quad \longleftarrow \quad \text{conservation of mass/energy}$$

where  $t$  is time



# A mathematical definition

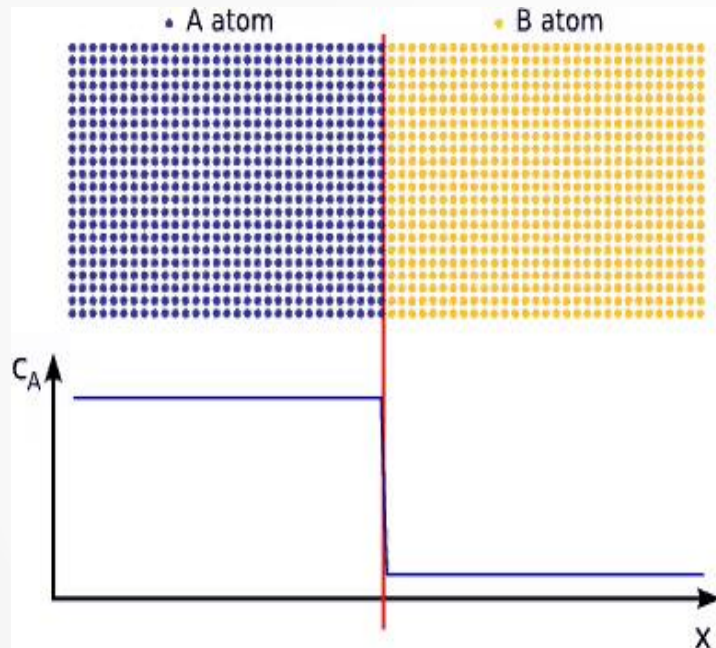
- How is  $\frac{\Delta C}{\Delta t} = -\frac{\Delta q}{\Delta x}$  a conservation of mass/energy equation?
- Consider the fluxes  $q_1$  and  $q_2$  at two points,  $x_1$  and  $x_2$

$$\frac{\Delta C}{\Delta t} = -\frac{q_2 - q_1}{x_2 - x_1}$$

What happens when the flux of mass  $q_2$  at  $x_2$  is larger than the flux  $q_1$  at  $x_1$ ?



# A mathematical definition



<http://web.unideb.hu/zerdelyi/>

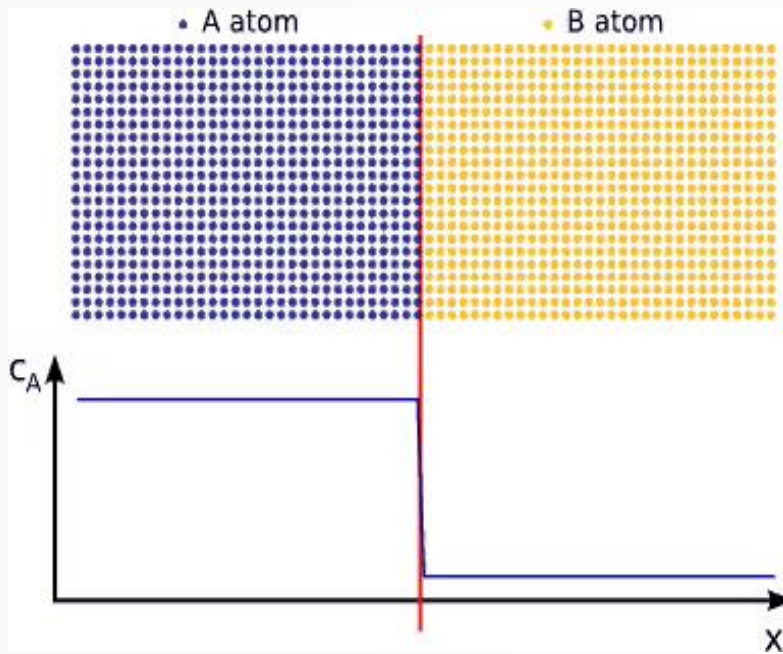
- Replace the finite changes  $\Delta$  with infinitesimal changes  $\partial$ , we can describe our example on the left

$$\frac{\delta C}{\delta t} = - \frac{\delta q}{\delta x}$$

→ The concentration of A will change based on the flux across a reference face at position  $x$  minus the flux across a reference face at position  $x + dx$



# A mathematical definition



<http://web.unideb.hu/zerdelyi/>

- In the exercise for this week we will explore some simple models for diffusion and some of the factors we need to consider



**10 min break!**



**Up next: An introduction to Thermochronology**



# References

- Zhang, K., Song, H., Chen, J., Geng, M., Liu, B. (2023). Gas Seepage Detection and Gas Migration Mechanisms. In: Chen, D., Feng, D. (eds) South China Sea Seeps. Springer, Singapore. [https://doi.org/10.1007/978-981-99-1494-4\\_3](https://doi.org/10.1007/978-981-99-1494-4_3)
- S M Aufrère, G Williams-Jones, S Moune, D J Morgan, N Vigouroux, J K Russell, Olivine Time-Capsules Constrain the Pre-Eruptive History of Holocene Basalts, Mount Meager Volcanic Complex, British Columbia, Canada, *Journal of Petrology*, Volume 65, Issue 9, September 2024, egae089, <https://doi.org/10.1093/petrology/egae089>
- Seonggan Jang, Changmin Kim, Heejun Suk, Minjune Yang, Assessing the persistence of a contaminant plume generated by linear aquifer source depletion and back diffusion from an aquitard, *Journal of Hazardous Materials*, Volume 480, 2024, 136021, ISSN 0304-3894, <https://doi.org/10.1016/j.jhazmat.2024.136021>.
- Shuster, D. L., Flowers, R. M., & Farley, K. A. (2006). The influence of natural radiation damage on helium diffusion kinetics in apatite. *Earth and Planetary Science Letters*, 249(3-4), 148–161.