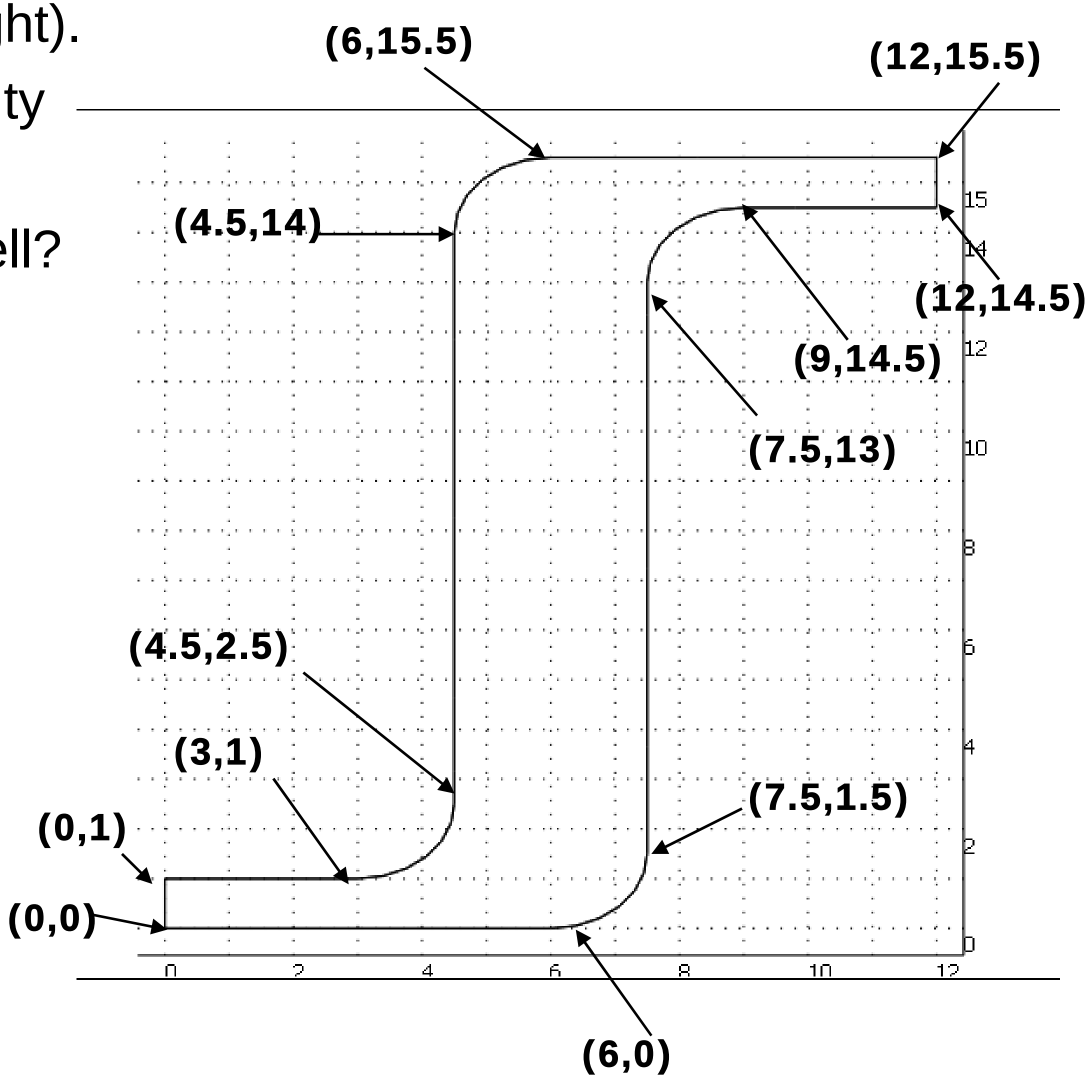
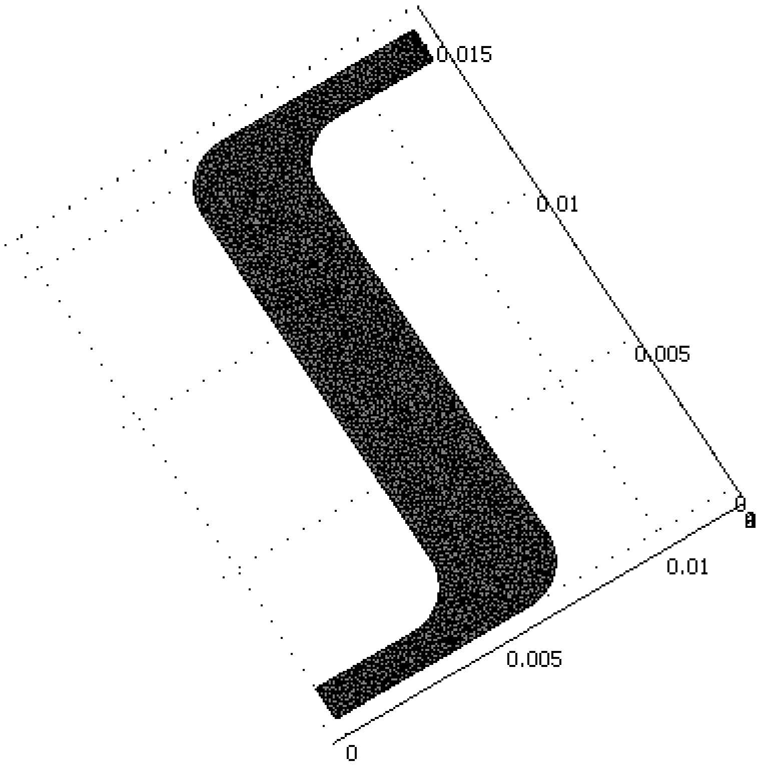
S-cell Problem (home work)

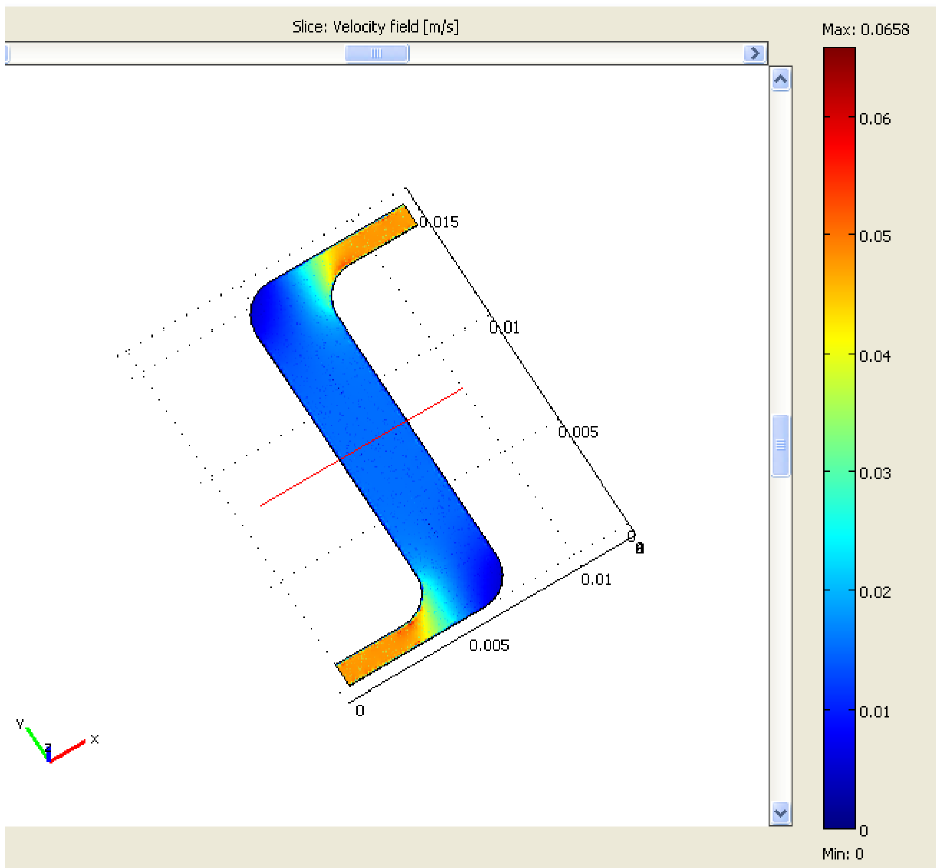
- Calculate velocity field in an S-cell (3D fluidic cell, 50µm height).
- What would flow field uniformity across a 1mmx1mm array

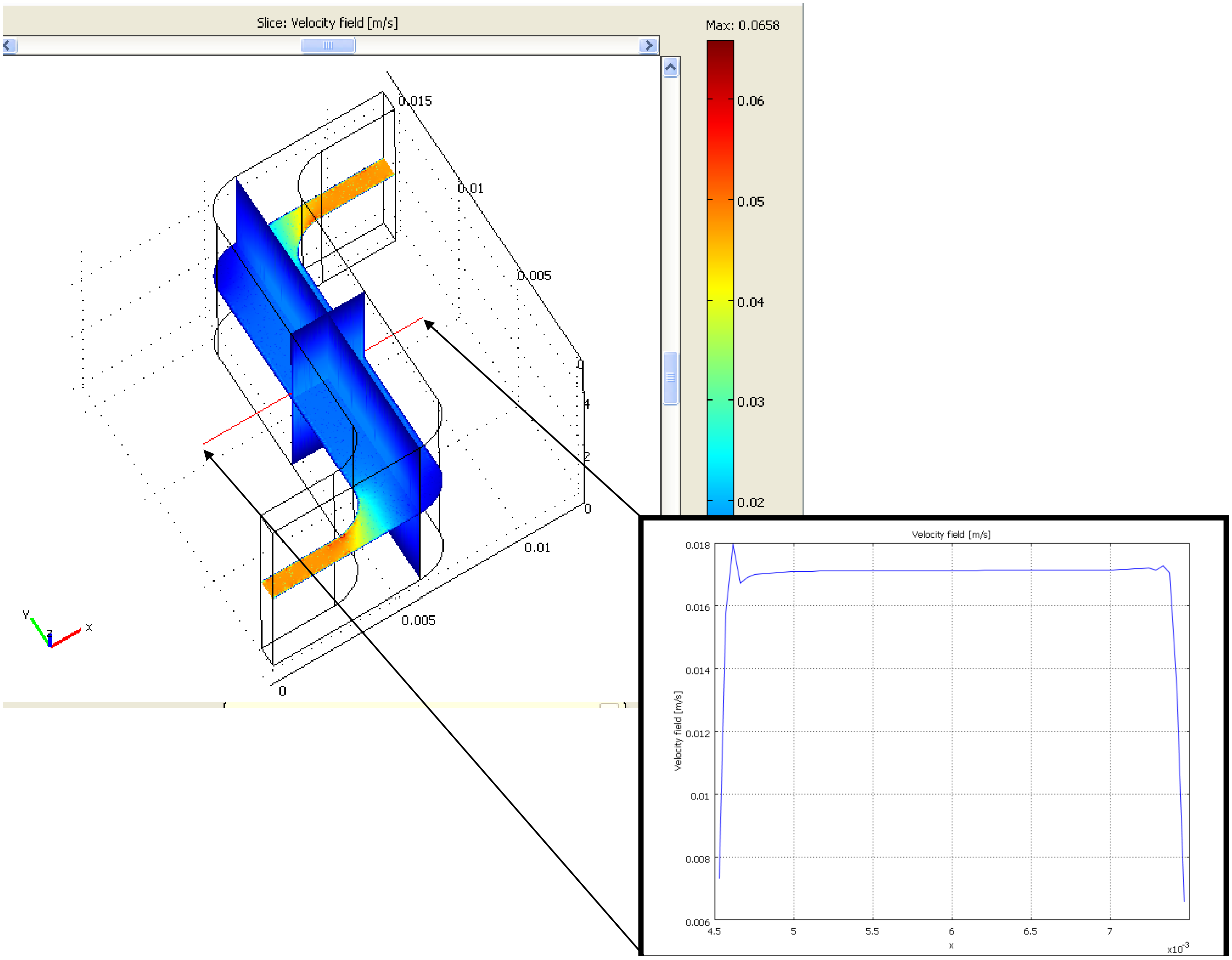
  spotted in the middle of the cell?



Data:
Flow rate: 100ul/min
Liquid: water, T=298K
Channel height (z): 50um
Channel width: 1mm in/outlet; 3mm chamber
Curvature radius: 1.5mm


0.015
0.01
0.005
0
0.01
0.005
0


Slice: Velocity field [m/s]
Max: 0.0658
0.06
0.05
0.04
0.03
0.02
0.01
0
Min: 0
0.015
0.01
0.005
0.01
0.005
0
y
x



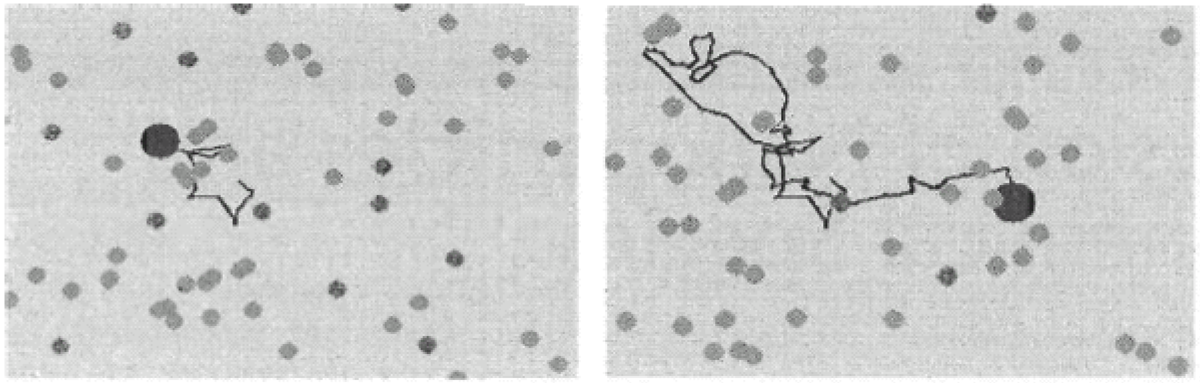
Slice: Velocity field [m/s]
Max: 0.0658
0.06
0.05
0.04
0.03
0.02
0.015
0.01
0.005
0
0.01
0.005
0
y
x
z
Velocity field [m/s]
0.018
0.016
0.014
0.012
0.01
0.008
0.006
4.5
5
5.5
6
6.5
7
x
x10-3
Velocity field [m/s]

Lecture 7

Flow and Diffusion. Micromixers. Multiphysics modelling with COMSOL

Brownian motion

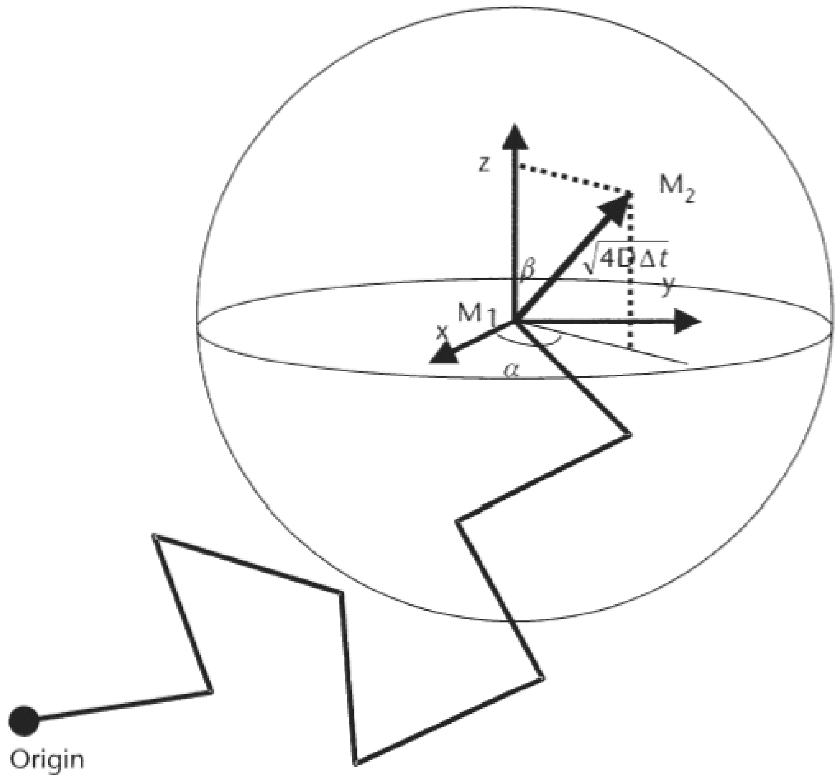
- discovered by R. Brown and J.Ingenhous by observation of pollen grains floating on water

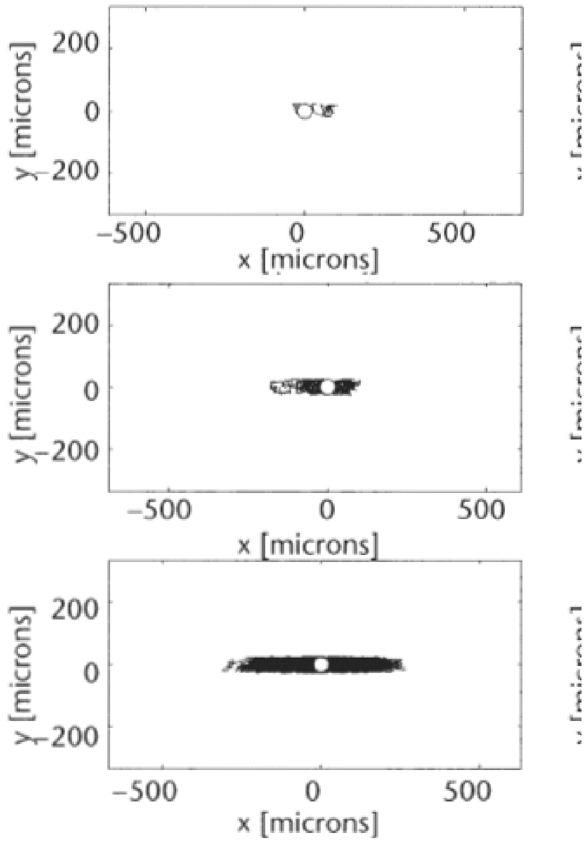


- macroscopic (concentration) and microscopic approach to diffusion

Random walk

- Diffusion can be modeled as a random walk using Monte-Carlo simulation





Microscopic approach

- Model: 1D random walk on a grid (uncorrelated steps left and right with constant step length ***l***)

$$\left\langle \Delta x_i \cdot \Delta x_j \right\rangle = l\delta_{ij}$$

- Average distance after N steps (averaged over M walks):

$$\left\langle \Delta x_N \right\rangle = \frac{1}{M}\sum_{j=1}^{M} x_N^{(j)} = \frac{1}{M}\sum_{j=1}^{M}\sum_{i=1}^{N} x_i^{(j)} = \sum_{i=1}^{N}\left\langle x_i \right\rangle = 0$$

- Rms distance after N steps (averaged over M walks):

$$\left\langle \Delta x_N^2 \right\rangle = \frac{1}{M}\sum_{j=1}^{M}\left[x_N^{(j)}\right]^2 = \frac{1}{M}\sum_{j=1}^{M}\left(\sum_{i=1}^{N} x_i^{(j)}\right)\left(\sum_{k=1}^{N} x_k^{(j)}\right) =$$

$$= \frac{1}{M}\sum_{j=1}^{M}\left(\left(\sum_{i=1}^{N}\left[x_i^{(j)}\right]^2\right) + \left(\sum_{i=1}^{N}\sum_{k\neq i}^{N} x_i^{(j)} x_k^{(j)}\right)\right) = Nl^2 + \overbrace{\sum_{i=1}^{N}\sum_{k\neq i}^{N}\left\langle x_i^{(j)} x_k^{(j)}\right\rangle}^{=0}$$

Microscopic approach (cont)

- Rms distance after N steps

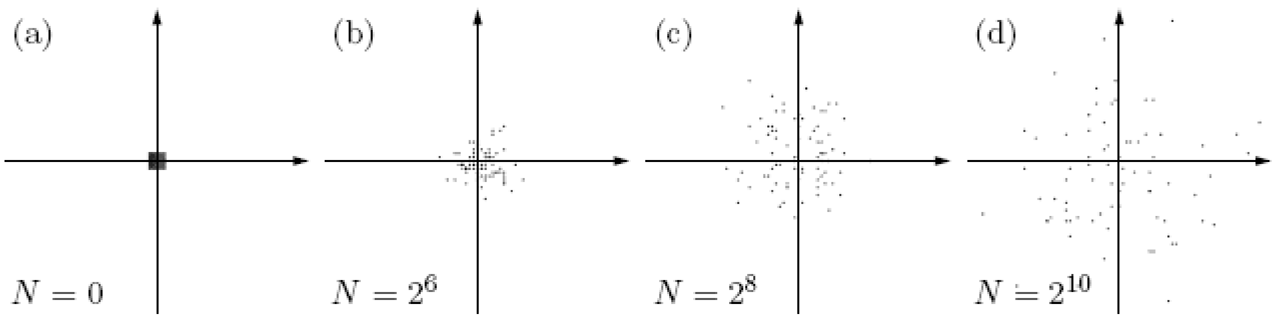
$$\left\langle \Delta x_N^2 \right\rangle = Nl^2$$

$$l_{diff,N} = \sqrt{\left\langle \Delta x_N^2 \right\rangle - \left\langle \Delta x_N \right\rangle^2} = \sqrt{N}\, l = \sqrt{\frac{tl^2}{\tau}} = \sqrt{Dt}$$

- In case of uncorrelated 2D steps

$$\left\langle R_N^2 \right\rangle = \left\langle x_N^2 + y_N^2 \right\rangle = \left\langle x_N^2 \right\rangle + \left\langle y_N^2 \right\rangle = 2Nl^2$$

$$l_{diff}^{2D} = \sqrt{2Dt}$$



Macroscopic approach to diffusion

- First Fick's law

$$J = -D\nabla c$$

- Second Fick's law

$$\frac{\partial c}{\partial t} = D\Delta c$$

$$\frac{\partial c}{\partial t} = D\Delta c - v\nabla c + S$$

source/sink term

- Einstein formula

$$D = \frac{kT}{C_D} \qquad D = \frac{kT}{6\pi\eta R}$$

Convection-diffusion equation

- Continuity equation for heterogeneous fluid

$$\frac{\partial \rho}{\partial t}+\nabla\left(\rho\vec{v}\right)=0;\quad \rho(\vec{r})\equiv\sum_{a}\rho_{\alpha}(\vec{r});\; C_{\alpha}(r,t)\equiv\frac{\rho_{\alpha}(r,t)}{\rho(r,t)}$$

- in integral form

Gauss theorem

$$\int_{\Omega}\frac{\partial C_{\alpha}\rho}{\partial t}dV=-\int_{\partial\Omega}n\cdot(C_{\alpha}\rho\vec{v}(r,t)+\vec{J}_{\alpha}^{diff})da=-\int_{\Omega}\nabla\cdot(C_{\alpha}\rho\vec{v}(r,t)+\vec{J}_{\alpha}^{diff})dV$$

$$\frac{\partial C_{\alpha}\rho}{\partial t}=\nabla\cdot(C_{\alpha}\rho\vec{v}(r,t)+\vec{J}_{\alpha}^{diff})$$

$$\rho\left[\frac{\partial C_{\alpha}\rho}{\partial t}+\vec{v}\cdot\nabla C_{\alpha}\right]=-\nabla\cdot\vec{J}_{\alpha}^{diff}$$

$$\frac{\partial C_{\alpha}}{\partial t}+\vec{v}\cdot\nabla C_{\alpha}=D_{\alpha}\nabla^{2}C_{\alpha}$$

convection-diffusion equation

Diffusion equation

- diffusion equation $\frac{\partial c}{\partial t} = D\nabla^2 c$

- from dimensional analysis $L_0 = \sqrt{DT_0}$

- Typical values:

$D \approx 2\cdot 10^{-9}\ \mathrm{m^2/s}$, small ions in water

$D \approx 5\cdot 10^{-10}\ \mathrm{m^2/s}$, sugar molecules in water

$D \approx 4\cdot 10^{-11}\ \mathrm{m^2/s}$, 30bp DNA in water

$D \approx 1\cdot 10^{-12}\ \mathrm{m^2/s}$, 5kbp DNA in water

Limited point-source diffusion

- Normal (Gaussian) distribution

$$P(s) \equiv \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}s^2}; \langle s \rangle = \int_{-\infty}^{\infty} sP(s)ds = 0; \langle s^2 \rangle = \int_{-\infty}^{\infty} s^2 P(s)ds = 1;$$

- Let's consider diffusion from a point source described by δ-function. $c(x,0) = N_0 \delta(x)$
The solution of the diffusion equation is:

$$c(x,t) = N_0 (4\pi Dt)^{-1/2} \exp\left[-\frac{x^2}{4DT}\right] = N_0 P(s_x),\ {s_x}^2 = \frac{x^2}{2Dt}$$

$$l^2{}_{diff} = \langle x^2 \rangle = 2Dt \langle {s_x}^2 \rangle = 2Dt$$

Limited point-source diffusion

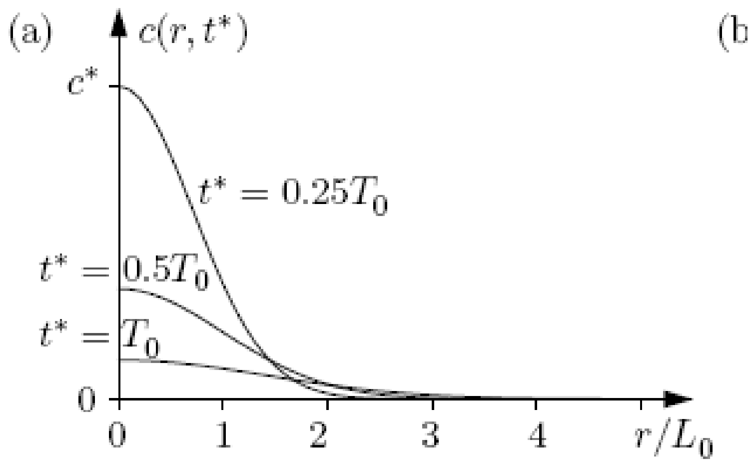
- In 2D case:

$$c(x,y,0) = N_0 \delta(x)\delta(y)$$

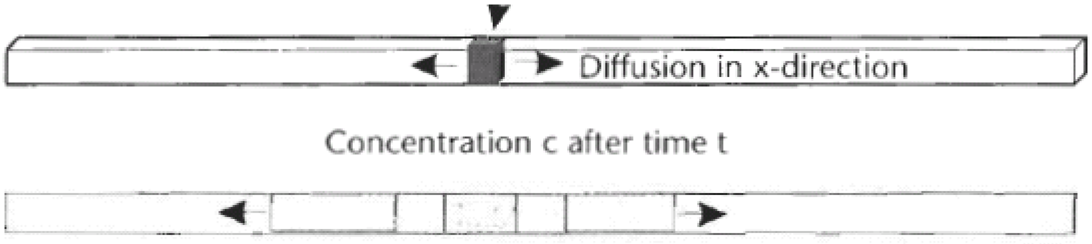
$$c(x,t) = N_0 (4\pi Dt)^{-1/2} \exp\left[-\frac{x^2}{4DT}\right] \times (4\pi Dt)^{-1/2} \exp\left[-\frac{y^2}{4DT}\right] =$$

$$= N_0 P(s_x) P(s_y)$$

$$l^2{}_{diff,2D} = \left\langle x^2 + y^2 \right\rangle = 2Dt \left\langle s_x{}^2 + s_y{}^2 \right\rangle = 4Dt$$

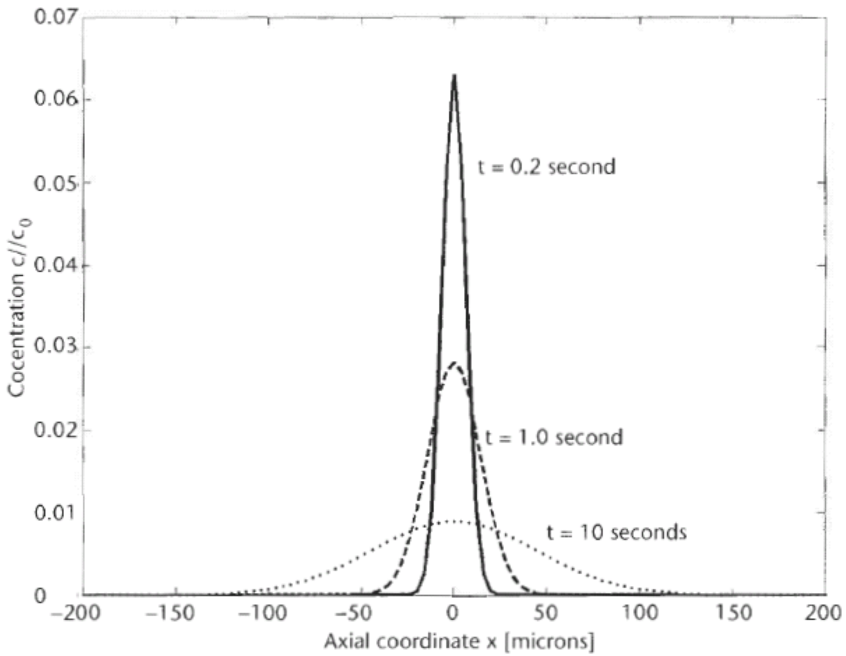


Spreading from a point source in 1D



- solution:

$$c(x,t) = \frac{c_0}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$



Limited planar source

- Let’s consider diffusion into half space.

$$c(r,0) = 2N_0\delta(x)$$

$$c(r,t) = N_0(\pi Dt)^{-1/2}\exp\left[-\frac{x^2}{4DT}\right] = 2N_0P(s_x),\ s_x{}^2 = \frac{x^2}{2Dt}$$

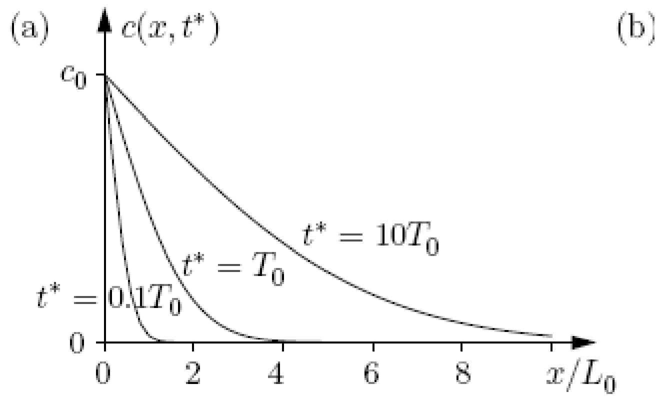
Constant planar source diffusion (Ilkovic's solution)

- Problem: consider a half-space with an initial concentration c_0. Concentration on the wall is zero at any time. Find the concentration profile vs time.

$$c = c_0 erf\left(\frac{x}{\sqrt{4Dt}}\right) \qquad erf(x) = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-u^2} du$$

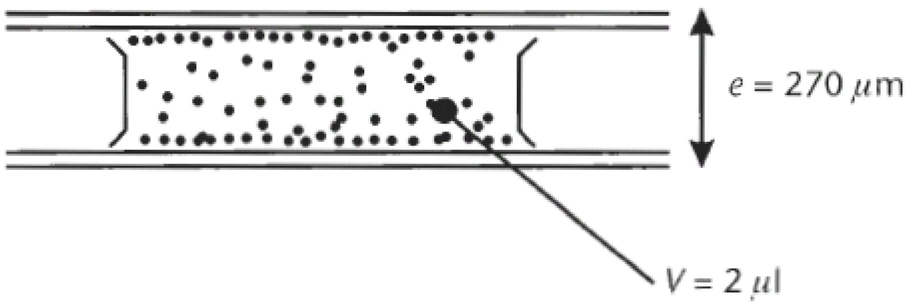
$$\frac{\partial c}{\partial x} = c_0 \frac{2}{\sqrt{\pi}} e^{-\frac{x^2}{4Dt}} \frac{1}{\sqrt{4Dt}}$$

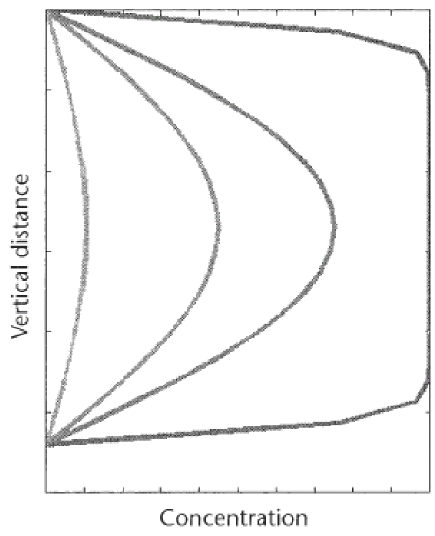
$$J = -D\nabla c_{|wall} = -c_0\sqrt{\frac{D}{\pi t}}$$



Example: diffusion between two plates

- A liquid drop contains nanoparticles that are immobilized upon contact with the walls. Find the concentration dependence vs time

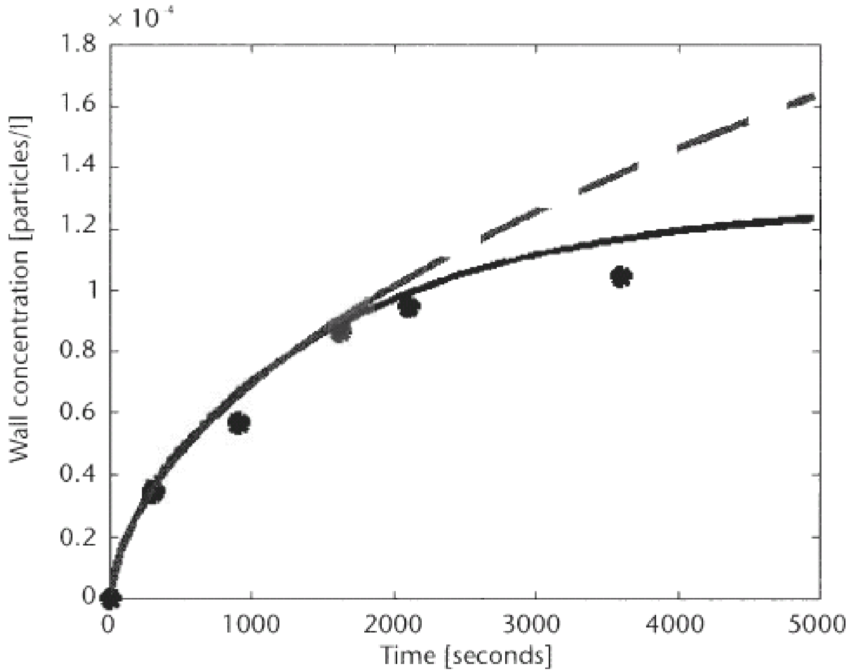




- For times less than $\tau = \dfrac{e/2}{4D}$

Ilkovic's solution can be used:

$$J = -2c_0\sqrt{\frac{D}{\pi t}}$$



Navier-Stokes equation: Diffusion of momentum

$$\rho \frac{\partial \vec{v}}{\partial t} = -\nabla p + \rho \vec{g} + \mu \nabla^2 \vec{v}$$

- In the case of decelerating Poiseuille flow

$$\frac{\partial \vec{v}}{\partial t} = \frac{\mu}{\rho} \nabla^2 \vec{v}$$

kinematic viscosity ν

Diffusion constant for momentum!

- Characteristic time for diffusion across the channel

$$T = \frac{a^2 \rho}{\mu}$$

$$\text{Schmidt number} = Sc = \frac{\nu}{D} = \frac{\mu}{\rho D}$$

intrinsic property of the solution

Diffusion vs Sedimentation

Does the gravity force affects the diffusion?

- Let's compare diffusion and sedimentation time across a microfluidic chamber

- sedimentation time:

$$C_D V_s = 6\pi\eta R_H V_s = \Delta\rho g \cancel{V}_p$$

$$V_s = \frac{2}{9}\frac{\Delta\rho g R^2}{\eta}$$

$$\tau_1 = d / V_s$$

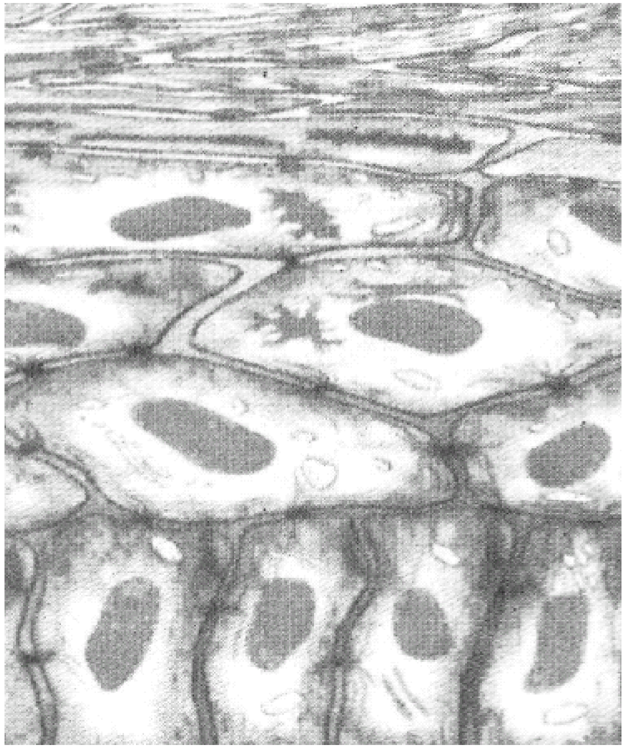
- diffusion time: $\tau_2 = \dfrac{d^2}{4D}$

$$\beta = \frac{\tau_1}{\tau_2} = \frac{d}{V_s}\frac{4D}{d^2} = 4\frac{kT}{\Delta mg}\frac{1}{d}$$

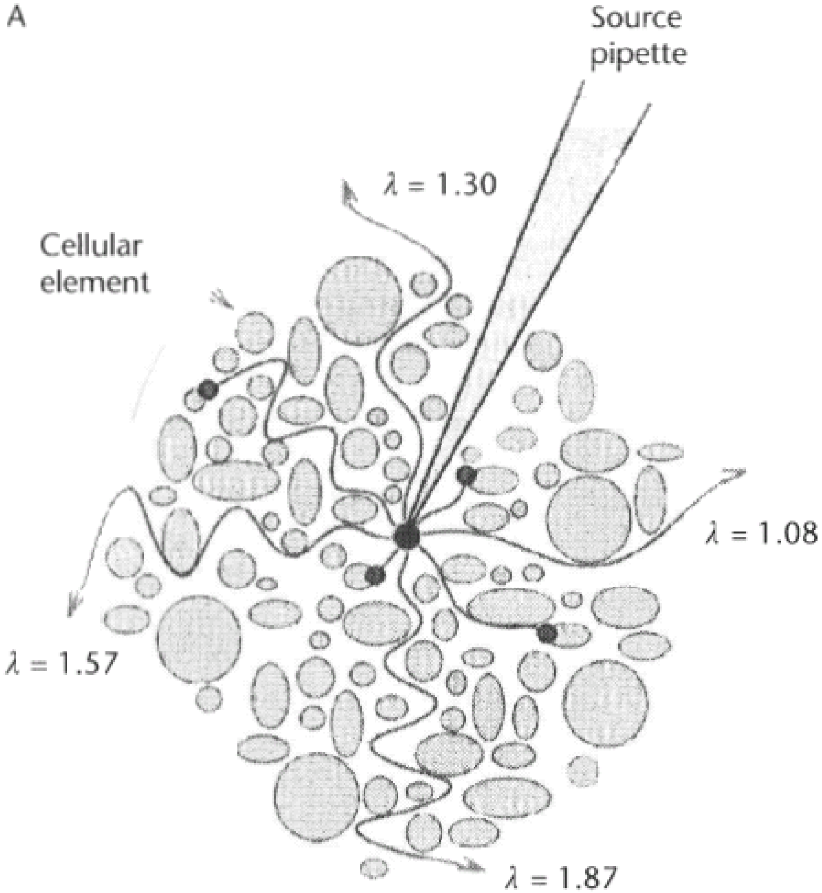
- if $\beta \ll 1$ sedimentation dominates

Diffusion in confined volumes

- For example, delivery of drugs relies on a diffusion in ECS of cellular clusters



cell arrangement in the human skin

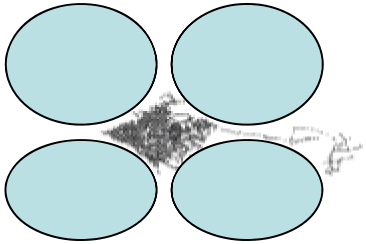


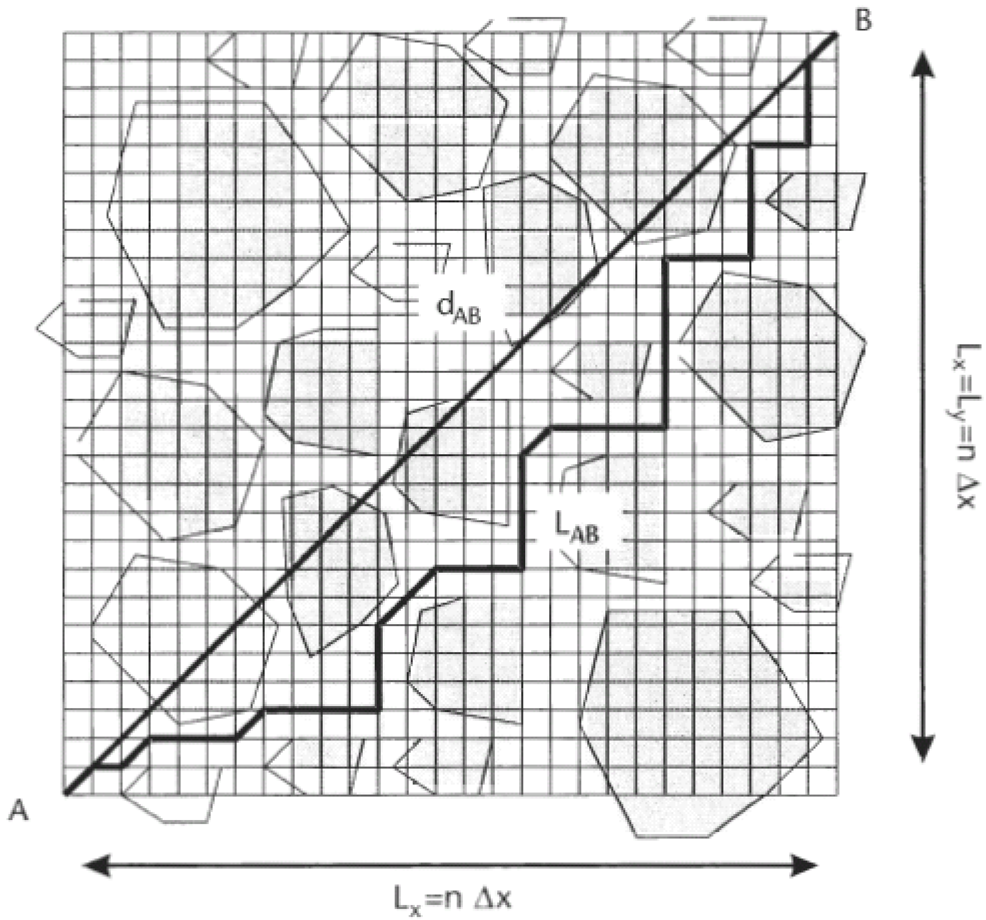
- tortuosity: ration between the distance in liquid and the straight distance between the points

Diffusion in confined volumes

It can be shown that:

- for any 2D regular isotropic lattice tortuosity is equal to $\tau = \sqrt{2}$
- for 3D: $\tau = \sqrt{3}$
- The situation is more complicated for irregular cells and in the presence of intercleft volumes

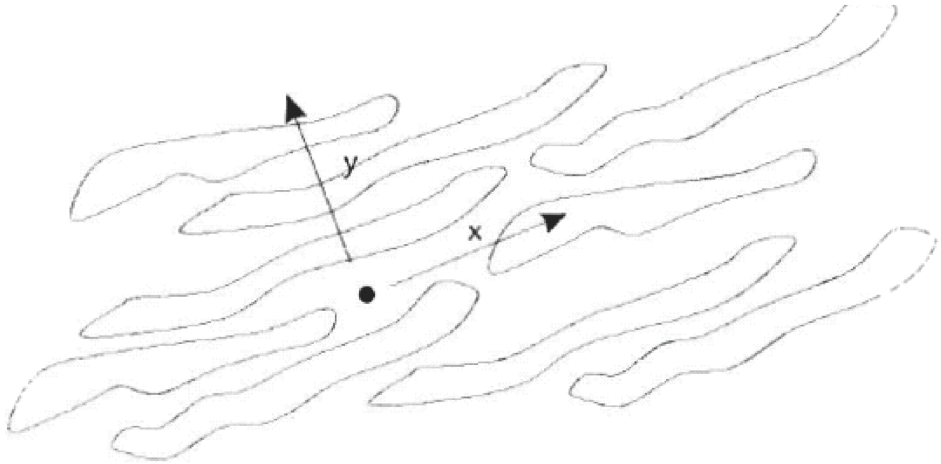




How to treat anisotropic media

- to treat a media with a preferential direction we have to introduce a diffusion tensor:

$$[D] = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}$$



$$\begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix} = -[D]\nabla c$$

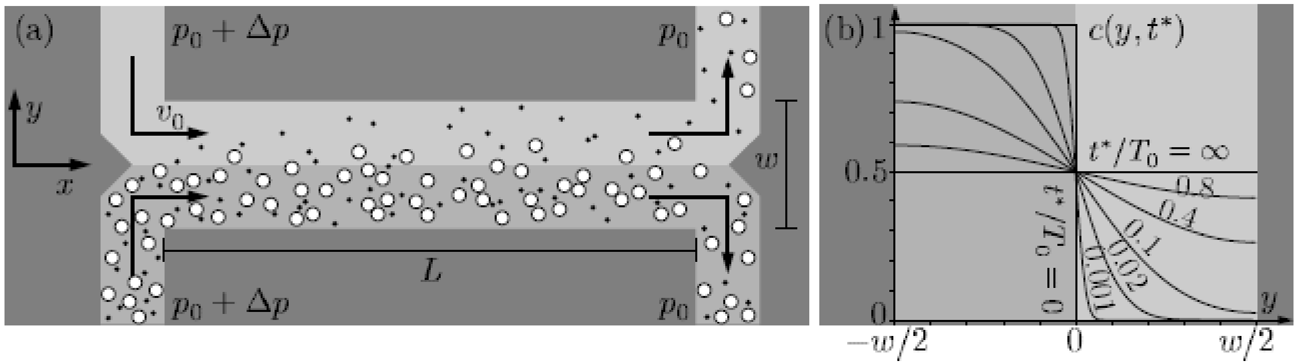
$$\frac{\partial c}{\partial t} = D_{11}\frac{\partial^2 c}{\partial x^2} + D_{22}\frac{\partial^2 c}{\partial y^2} + D_{33}\frac{\partial^2 C}{\partial z^2} + (D_{23} + D_{32})\frac{\partial c}{\partial y \partial z}$$

$$+(D_{31} + D_{13})\frac{\partial c}{\partial z \partial x} + (D_{12} + D_{21})\frac{\partial c}{\partial x \partial y}$$

- by rotating and scaling the coordinates it's possible to return to a isotropic (scalar) D:

$$\frac{\partial c}{\partial t} = D\left[\frac{\partial^2 c}{\partial \xi^2} + \frac{\partial^2 c}{\partial \eta^2} + \frac{\partial^2 c}{\partial \zeta^2}\right]$$

H-filter: separating solutes by diffusion



- H-filter takes advantages of laminar flow (flow don't mix) and fast diffusion over short distances

- Characteristic times:

convection time: $$\tau_{conv} = \frac{L}{v_0}$$

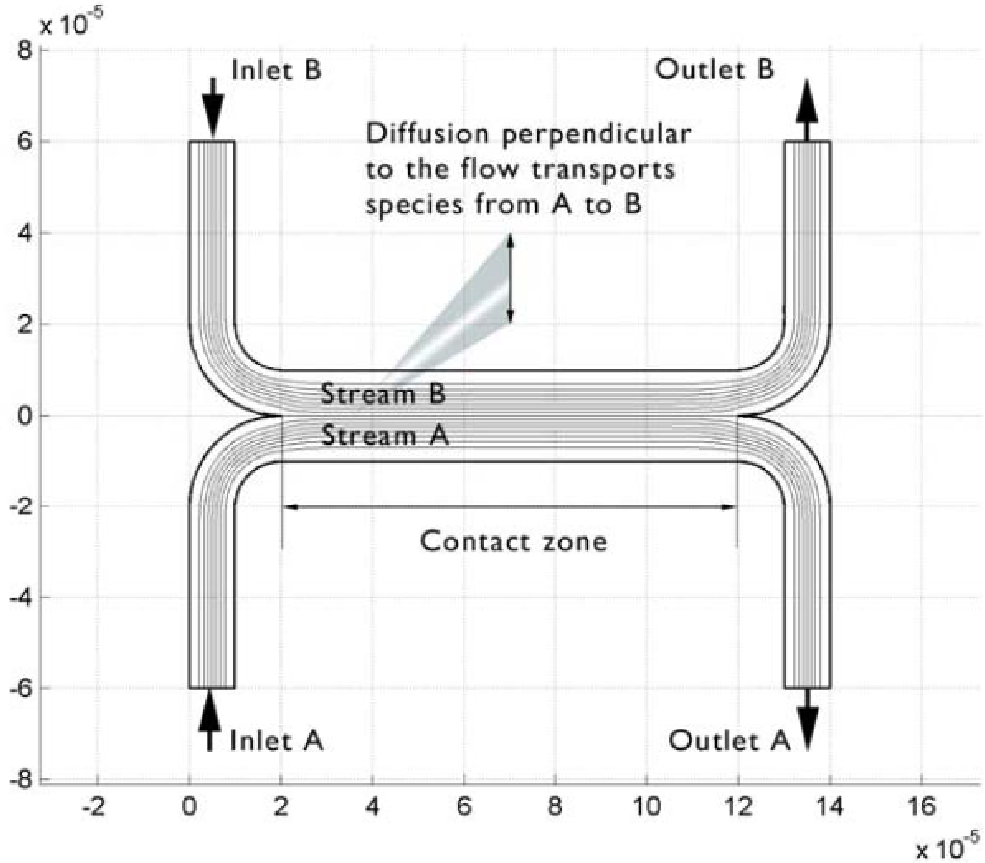
diffusion time: $$\tau_{diff} = \frac{w^2}{4D}$$

$$\tau_{conv} \geq \tau_{diff}$$ concentration of solute is the same through the channel

- Critical diffusion constant: $$D^* = \frac{v_0 w^2}{4L}$$

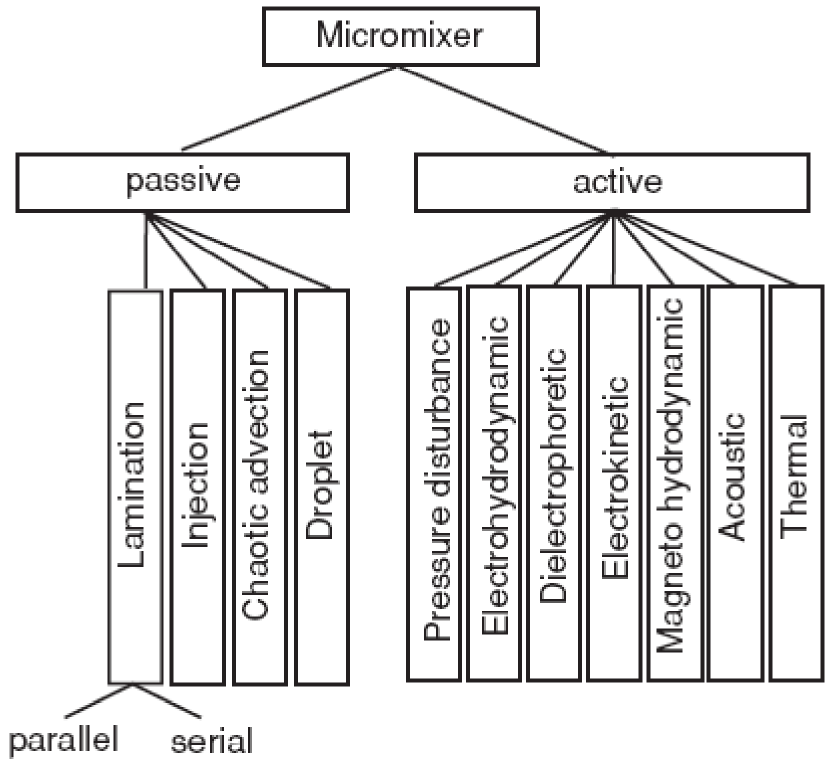
H-cell model

- H-cell perform separation via diffusion during controlled time:
  - Two laminar streams are brought into contact for given amount of time
- Small species from A can diffuse into B
- Modelling parameters:
  - Cell height – 20µm
  - Pressure at inlets: P_0=2 Pa;
- Calculate critical diffusion constant and compare with the modelling results



Mixing on microscale

- Flow in microchannels is laminar and mixing occurs through diffusion (slow!)
- Chemical reactions (necessary for Lab-on-Chip assays, but also for DNA and protein synthesis etc.) require mixing of reagents

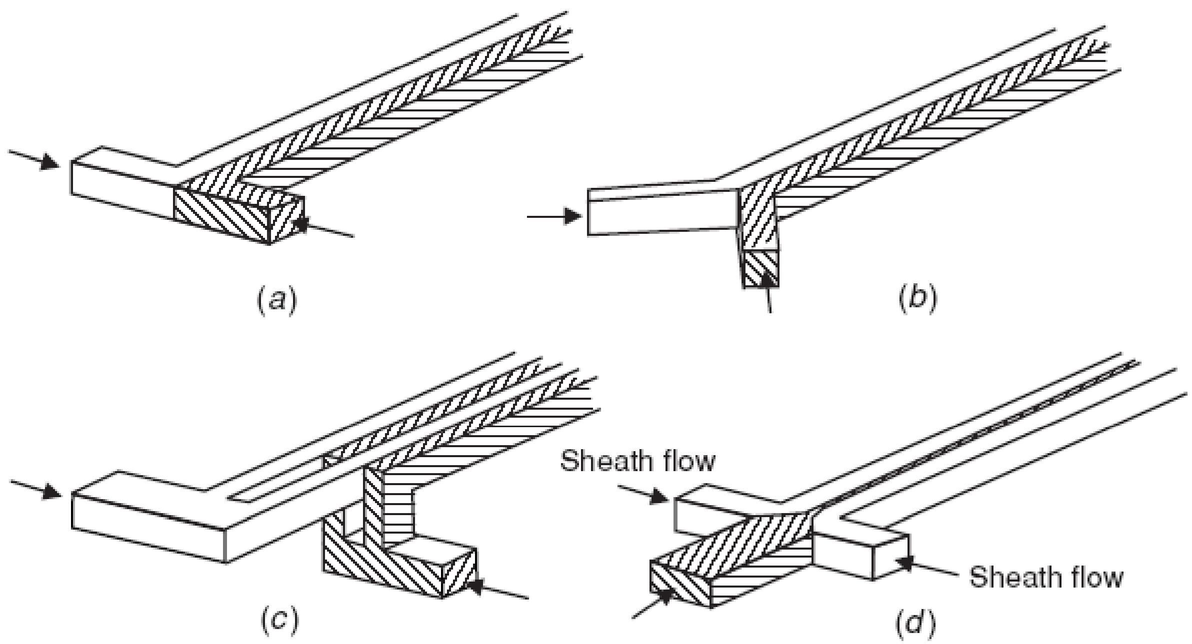


Passive micromixers

- General approach: to shorten diffusion time via increased contact/decreased thickness or by chaotic advection

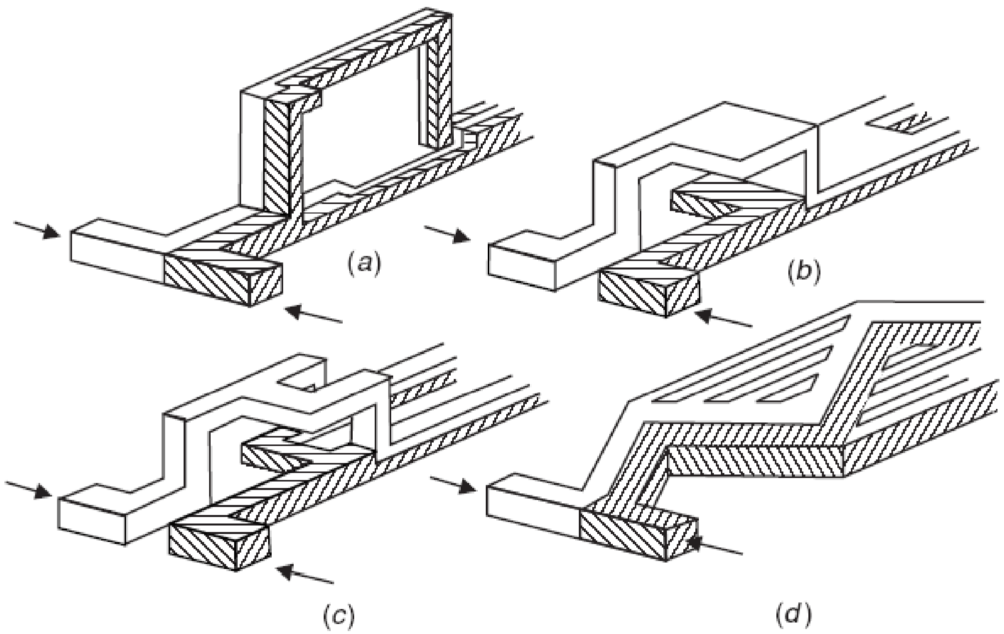
---

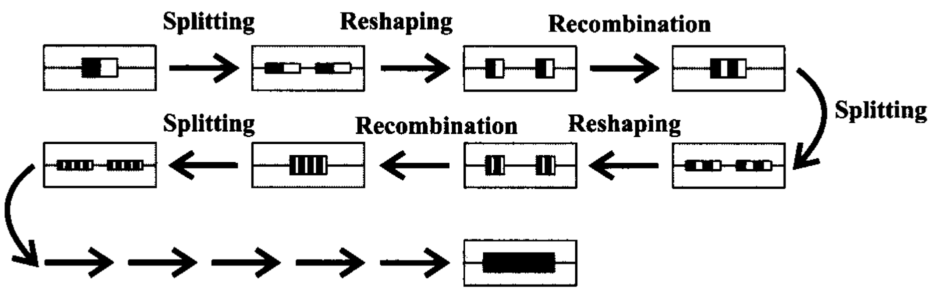
- Parallel lamination:



Passive micromixers

- Serial lamination:

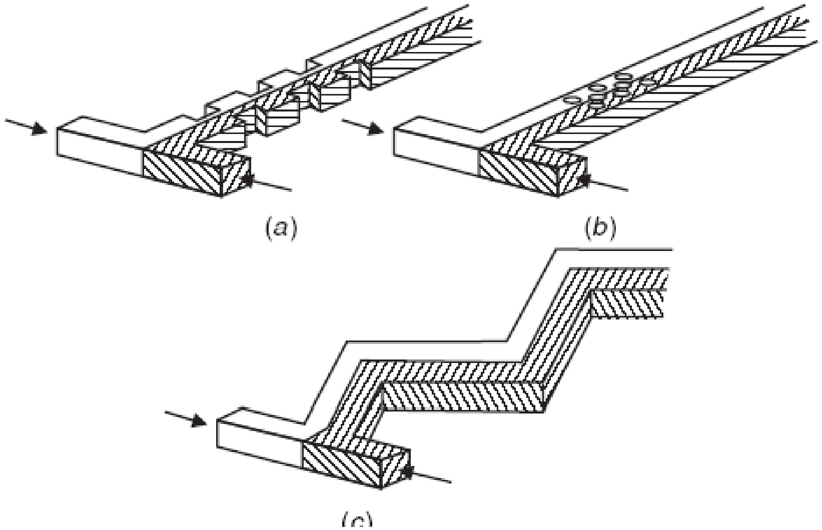




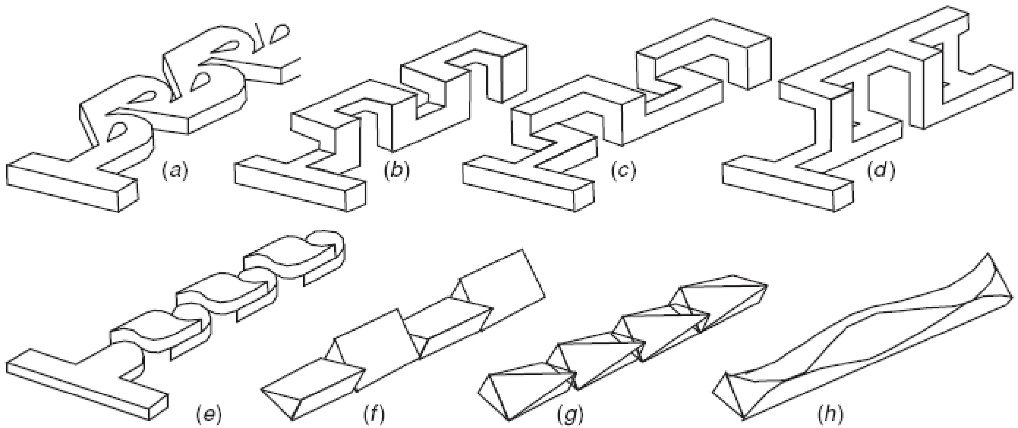
Passive micromixers

- Chaotic advection at high Re numbers

Recirculation are produced at the zig-zag turns of channel or behind the obstacles. Critical Re numbers are reported ~80 for zig-zag channel

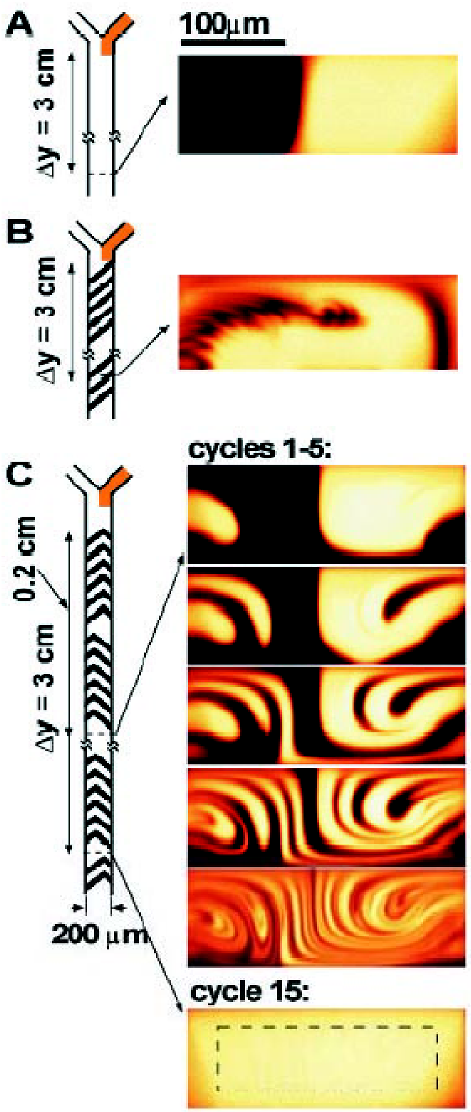


- Chaotic advection at intemediate Re numbers



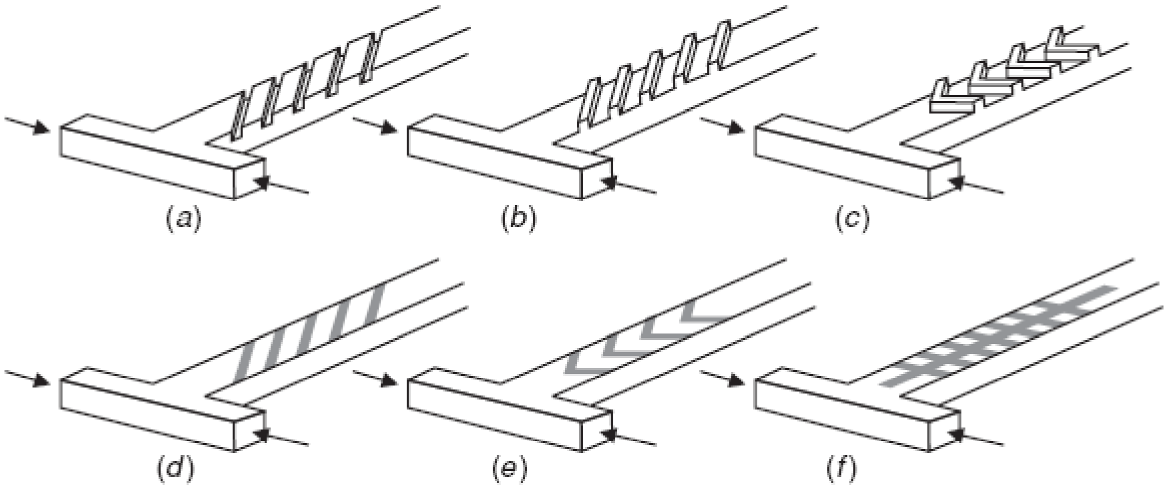
Passive micromixers

- Another way to induce mixing in laminar flow – patterned surface
  - Top -- no surface patterning
  - Middle – slants
  - Bottom V-shape (herringbone) – clearly see enhanced mixing
- Effective at low Reynolds numbers (in the range of 1- 100)



Passive micromixers

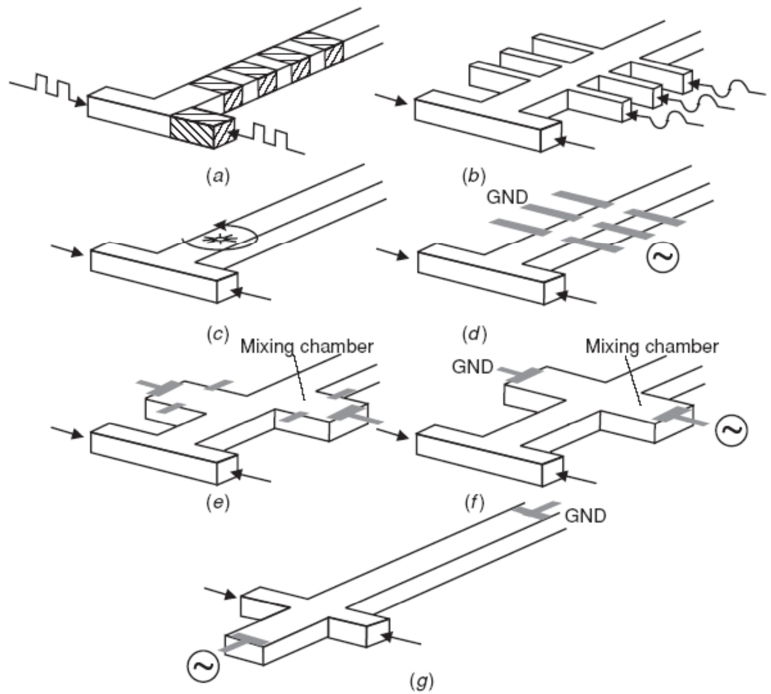
- Design variations of chaotic advection mixers



- Droplet micromixers

Active micromixers

- Function via
  - pressure disturbance,
  - mechanical microstirrers,
  - electrohydrodynamic
  - electrophoretic disturbance



Problems

- An analyte (c_a=1)is injected into S-cell. Plot concentration vs. time in the middle of the cell. How concentration is varied across the 1mm central area?
- Problems 5.7 and 5.8 (Bruus).