Diffusion challenges in (chemical) industries

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Diffusion Fundamentals II
27.08.07
L'Aquila, Abruzzi, Italia

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The many contexts of diffusion...

...@ DiffuFu-II:

•Talks Cavalli-Sforza, Vogl

•Poster B9 (Fujie, Odagaki)

...@ in economic life: ...

Limiting the topic a bit...

... Fickian and near-Fickian diffusion of molecules and/or energy

Outline

- Scaling behaviour of diffusion effects
- Diffusion as a challenge:
  - Diffusion of heat
  - Diffusion of reactants
  - Diffusion in multicomponent materials and finished goods
- Diffusion as a friend: controlled release
- Going micro and nano: approaching the apparent dwarf

Scaling behaviour of diffusion effects

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Macroworld experience: Diffusion is slow.

Typical example: a real Saxonian „Semester-uhr“ („term clock“)

Scaling behaviour of diffusion effects

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Nevertheless: sufficient change to observe during first hour of the experiment.

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Non-linear time behaviour of diffusion

... taking a closer look at the short-time behaviour...

Scaling behaviour of diffusion effects

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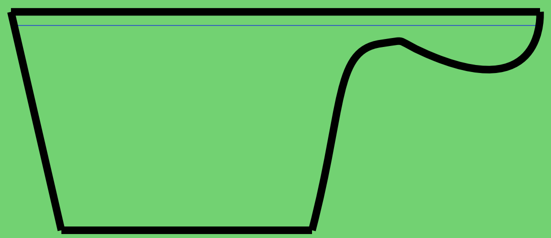
Dissolution of coloured ions: $KMnO_4$ and eosin



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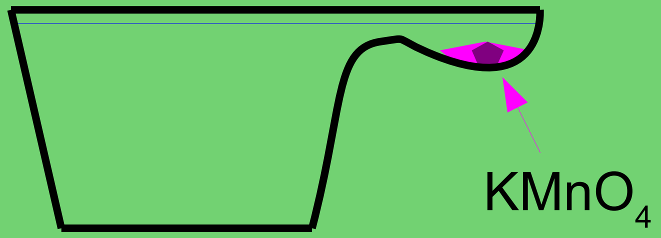

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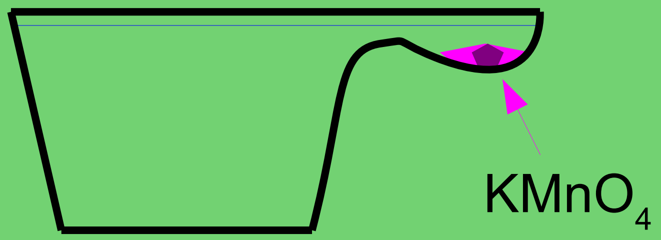

Dominating effect:
density-driven flow

Scaling behaviour of diffusion effects

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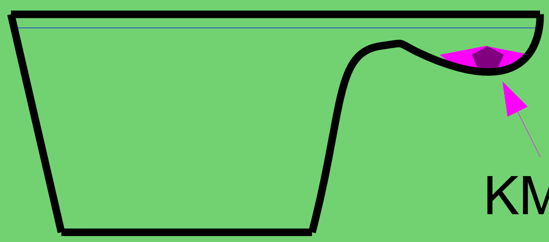

Xanthan gum, 0,5 % w/v dissolved in water (no major effect on diffusion)

Water

Dominating effect: density-driven flow

Suppression of convection by xanthan

Scaling behaviour of diffusion effects

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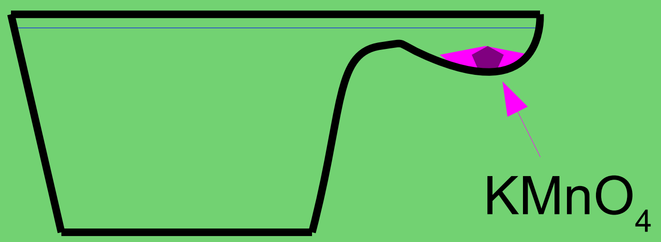

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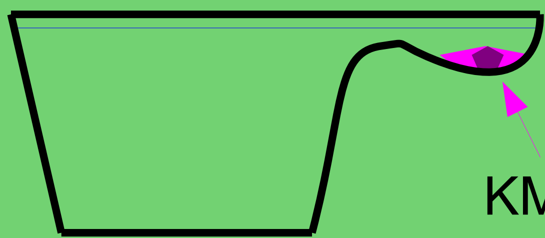
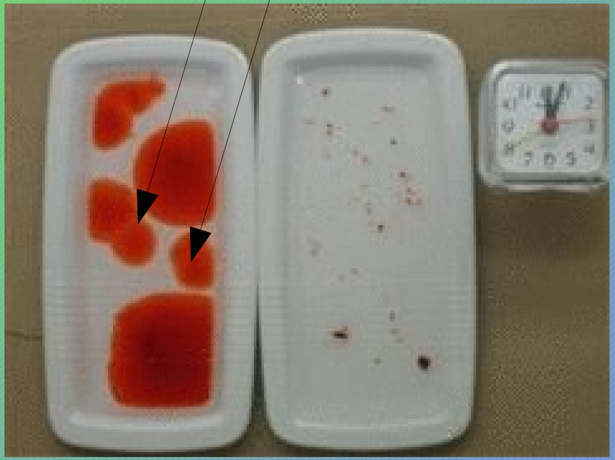


$KMnO_4$

Convection cells, „interference“



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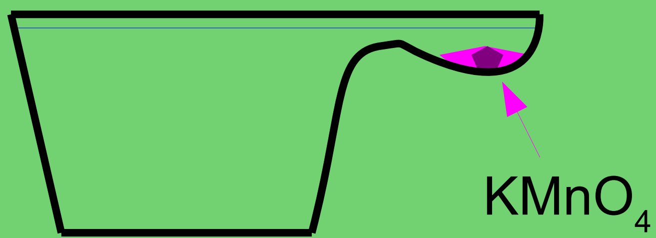

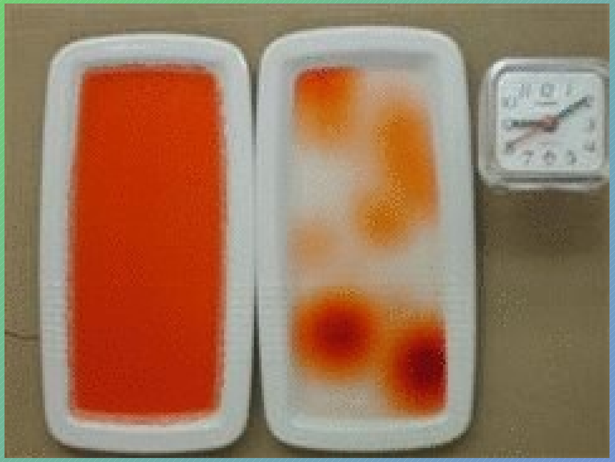

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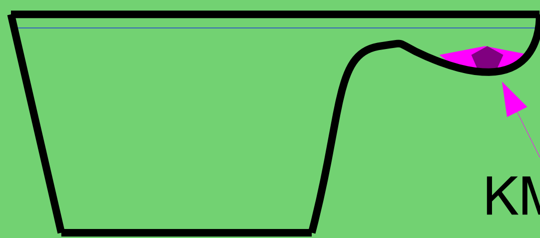
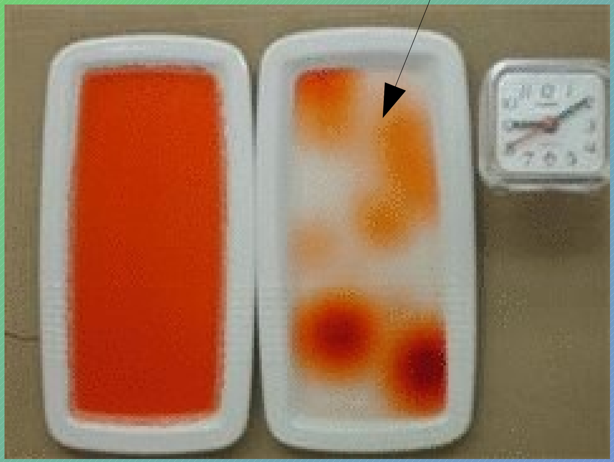


Diffuse concentration profiles, no „interference“



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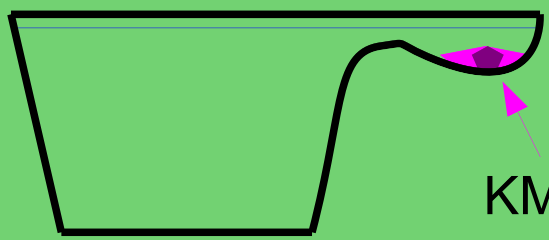
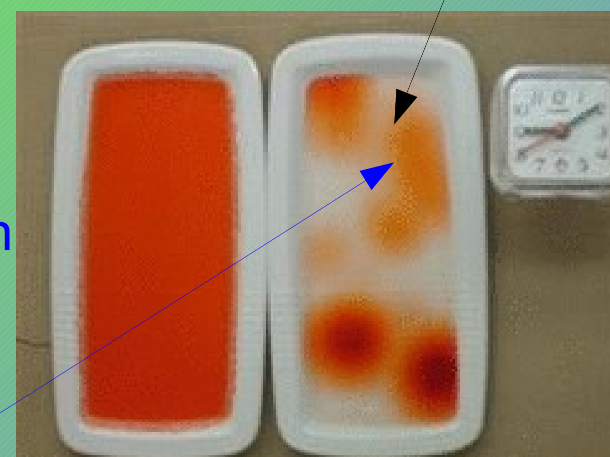


$KMnO_4$

Seemingly constant supply of dissolved $KMnO_4$

Diffuse concentration profiles, no „interference“

Propagation of eosin slows down with time



Dominating effect: density-driven flow

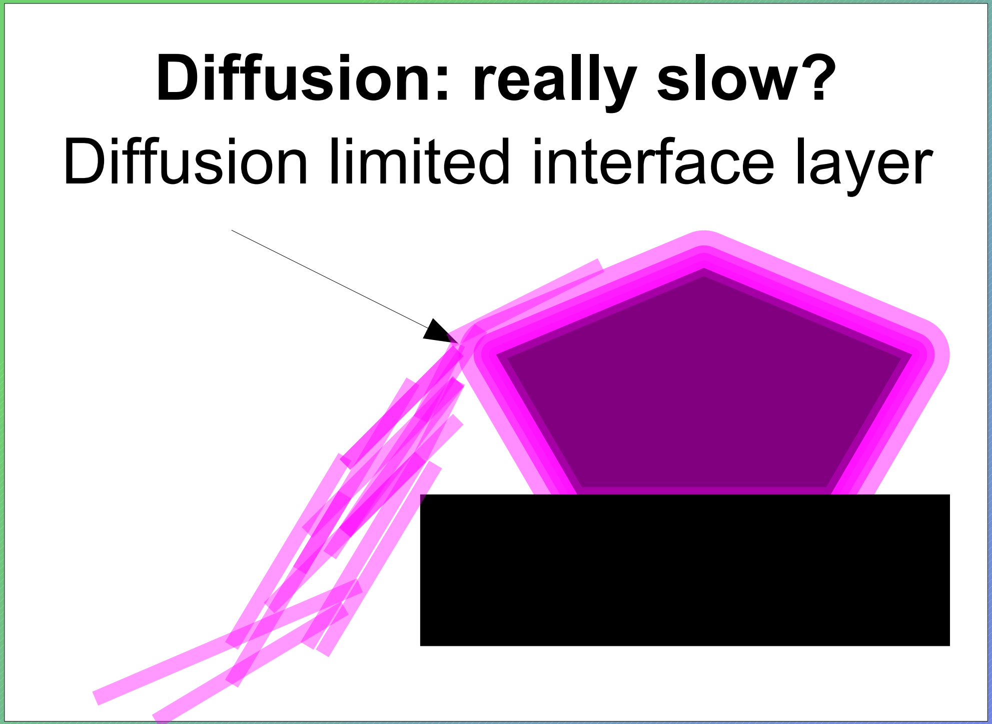
Suppression of convection by xanthan

Scaling behaviour of diffusion effects

Dissolution of coloured ions: $KMnO_4$ and eosin

Diffusion through thin stagnant layer at crystal-water interface allows fast mass transport into region of convective flow.

→ Fast convection on macroscale is fed by fast diffusion on micro-scale.



Scaling behaviour of diffusion effects

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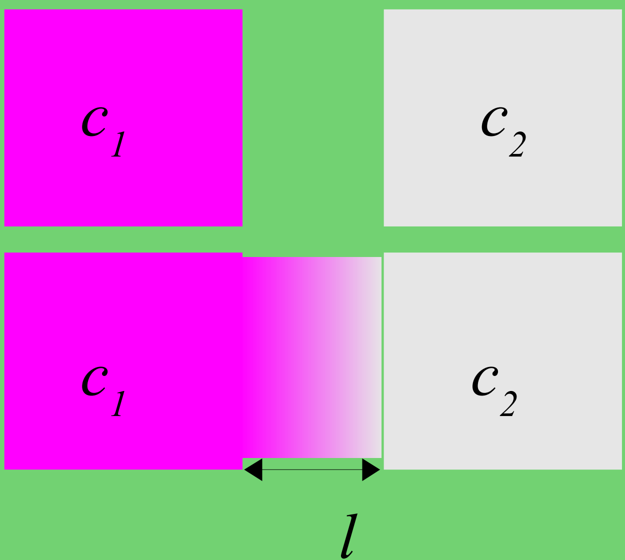
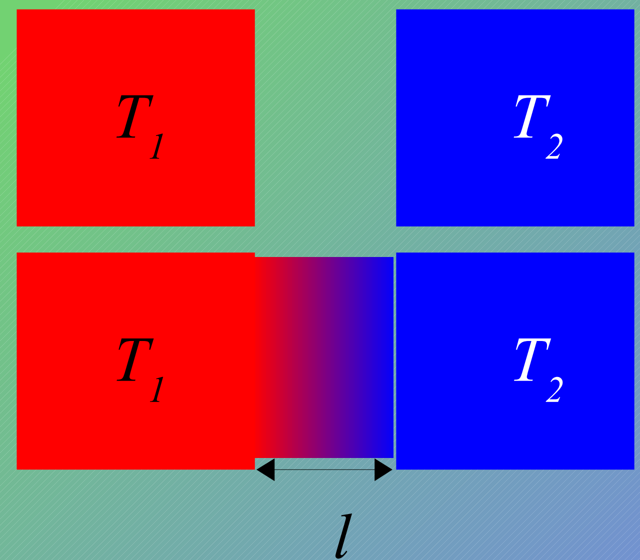
Fick's first law



Fourier's law



„Large“ reservoirs

Stationary profile of c or T in wall

Diffusive current through wall:

$$j_D = -D \frac{c_1 - c_2}{l}$$

$$j_D = -D \frac{dc}{dx}$$

$$j_Q = -\lambda \frac{T_1 - T_2}{l}$$

$$j_Q = -\lambda \frac{dT}{dx}$$

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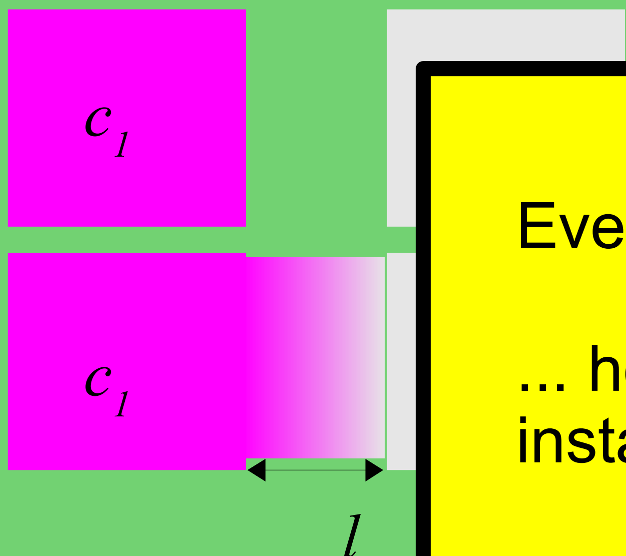

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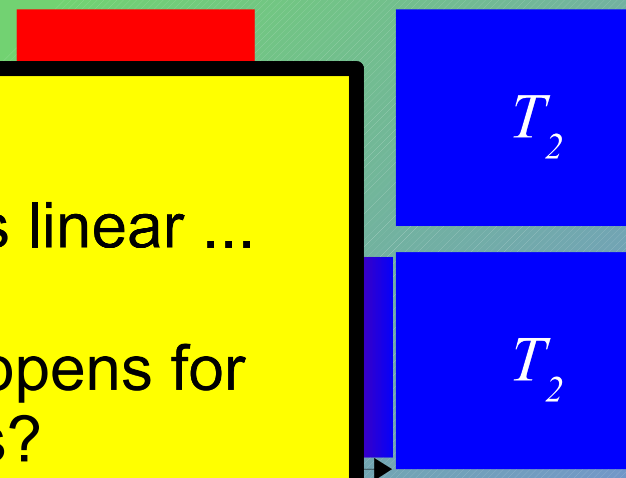

Everything still seems linear ...

... however: What happens for instationary situations?

$$j_D = -D\frac{c_1 - c_2}{l}$$

current through wall:

$$j_Q = -\lambda\frac{T_1 - T_2}{l}$$

$$j_D = -D\frac{dc}{dx}$$

$$j_Q = -\lambda\frac{dT}{dx}$$

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Example: instationary heat diffusion:
Heat current produces change in inner energy, i.e. heating of volume element:

$$dU = (j_Q(x) - j_Q(x+dx)\,A)\,dt$$

$$dU = C\,dm\,\frac{dT}{dt}\,dt = C\,\rho\,dV\,\frac{dT}{dt}\,dt = C\,\rho\,A\,dx\,\frac{dT}{dt}\,dt$$

Scaling behaviour of diffusion effects

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$$dU = Cdm\frac{dT}{dt}dt = C\rho\,dV\frac{dT}{dt}dt = C\rho\,Adx\frac{dT}{dt}dt$$

Comparing the expressions leads to

$$C\rho\,Adx\frac{dT}{dt}dt = (j_Q(x) - j_Q(x+dx))\,Adt$$

$$C\rho\frac{dT}{dt}dx = (j_Q(x) - j_Q(x+dx)) = -dj_Q(x)$$

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$$j_Q = -\lambda\frac{dT}{dx}$$

$$C\rho\frac{dT}{dt} = -\frac{dj_Q(x)}{dx} = \lambda\frac{d^2T}{dx^2}$$

Fick's second law of heat diffusion

Scaling behaviour of diffusion effects

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$$j_Q = -\lambda\frac{dT}{dx}$$

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2}$$

Fick's second law of (matter) diffusion

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Fick's second law of heat diffusion

Scaling behaviour of diffusion effects

Solution of diffusion equation for δ–shaped disturbance (1D):

$$c(x,t) = \frac{C_o}{2\sqrt{\pi D t}} \exp\left(\frac{-x^2}{4Dt}\right)$$

Mean diffusive shift:

$$s_{D,1D} = \sqrt{< x^2 >} = \sqrt{2Dt}$$

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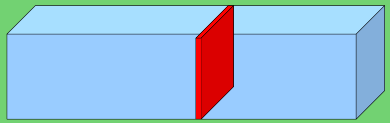

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into a 3D medium

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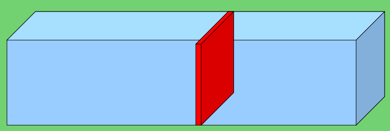
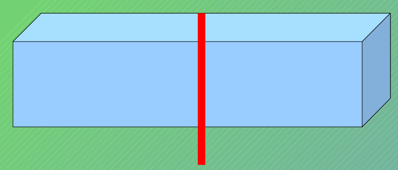


Diffusion from a line source

$$c(x,t)=\frac{M_o}{4\pi Dt}\exp\left(\frac{-x^2}{4\mathrm{Dt}}\right)$$



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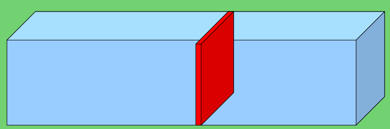

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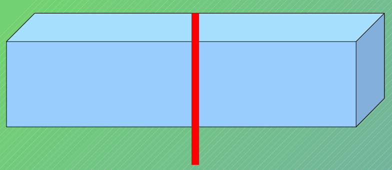
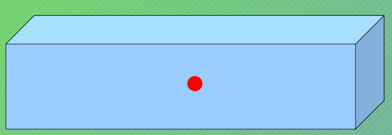


or a point source



$$c(x,t) = \frac{M_o}{8\left(\sqrt{\pi D t}\right)^3} \exp\left(\frac{-x^2}{4Dt}\right)$$

into a 3D medium

Scaling behaviour of diffusion effects

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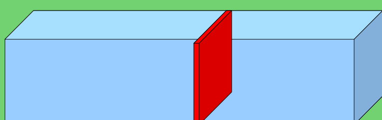

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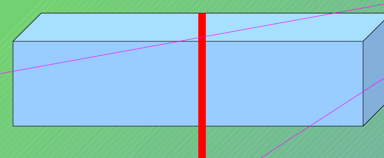

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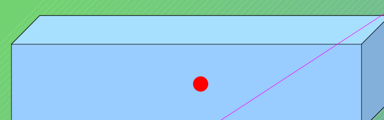


$$c(x,t)=\frac{M_o}{8(\sqrt{\pi Dt})^3}\exp\left(\frac{-x^2}{4Dt}\right)$$

Different normalization factors due to geometry: Faster depletion of concentration in center due to growing volume elements for cyclindrical and spherical geometry.

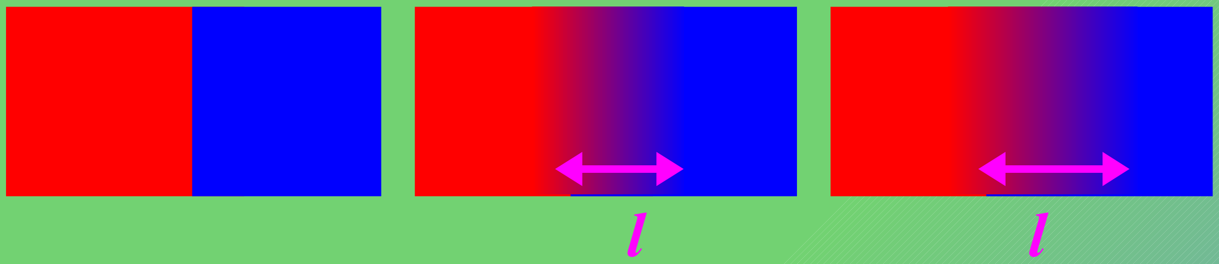
into a 3D medium

Scaling behaviour of diffusion effects

More realistic scenarioes: semiinfinite media and finite sheets

$$\frac{dT}{dt} = \frac{\lambda}{C\rho}\frac{d^2T}{dx^2} = \alpha\frac{d^2T}{dx^2}$$

$$\alpha = \frac{\lambda}{C\rho}$$ Heat diffusion coefficient



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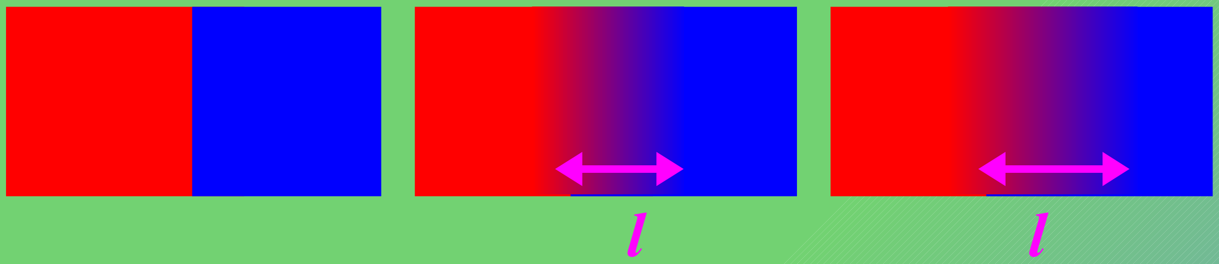

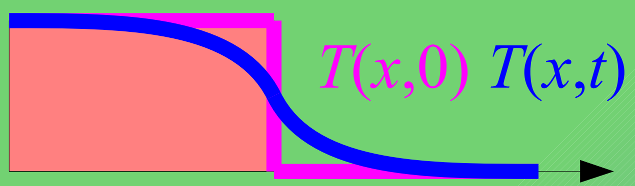

$$T(x,t)=\frac{1}{2}T_o\,erfc\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

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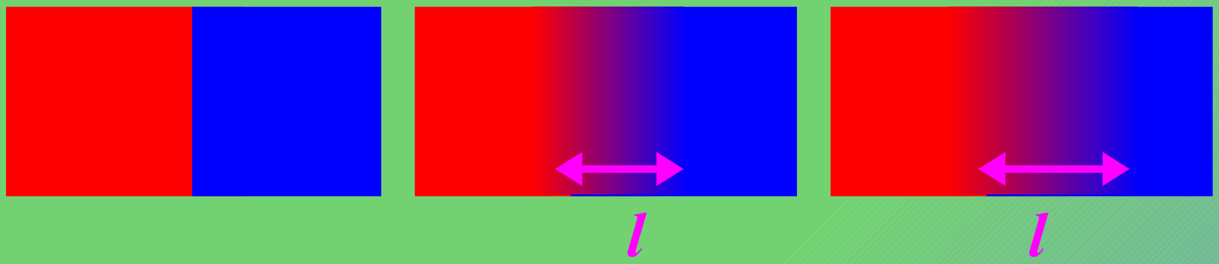

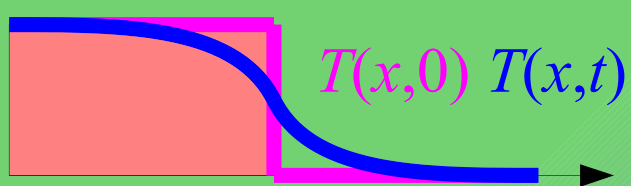

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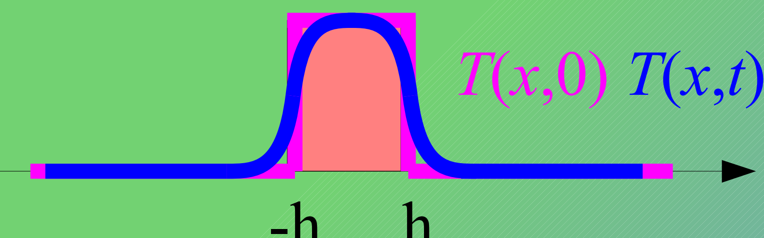

$$T(x,t)=\frac{1}{2}T_o\left[erf\left(\frac{h-x}{2\sqrt{\alpha t}}\right)-erf\left(\frac{h+x}{2\sqrt{\alpha t}}\right)\right]$$

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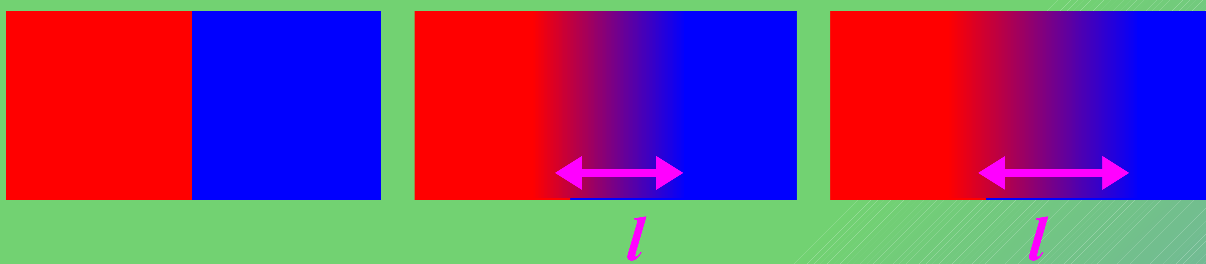
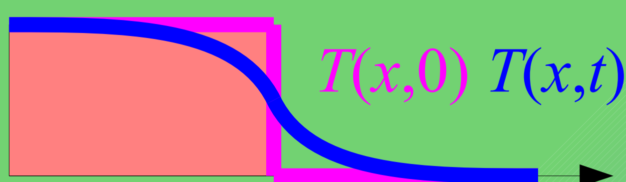
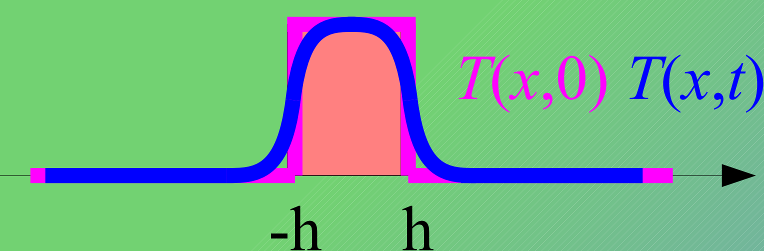


$$l \propto \sqrt{\alpha t}$$



$$T(x,t) = \frac{1}{2}T_o \, erfc\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

Relevant characteristic lenght scale for all diffusion processes



$$T(x,t) = \frac{1}{2}T_o\left[erf\left(\frac{h-x}{2\sqrt{\alpha t}}\right) - erf\left(\frac{h+x}{2\sqrt{\alpha t}}\right)\right]$$

Scaling behaviour of diffusion effects

„Velocity“ of diffusive transport processes:

$$v_D = \frac{s_D}{t_s} = \frac{s_D}{\frac{s_D^{\ 2}}{2D}} = \frac{2D}{s_D}$$

Inversely proportional to diffusion length!

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Inversely proportional to diffusion length!

Ratio of diffusive velocity to characteristic velocity in system:

$$\frac{v_{Char}}{v_D} = \frac{s_D v_{Char}}{2D}$$

Péclet number $\mathbf{Pe} = \frac{L_{Char} v_{Char}}{D}$

Scaling behaviour of diffusion effects

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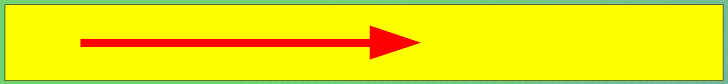
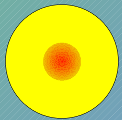
axial and radial





Diffusion as a challenge: Heat

Heating extended objects

e.g. baking

Chapati

almost homogeneous

baking time

< 1min

European-style bread

obviously inhomogeneous

baking time

> 1 h

Diffusion as a challenge: Heat

Heating extended objects

Heating up extended objects: intrinsically slow
(time- and energy consuming)

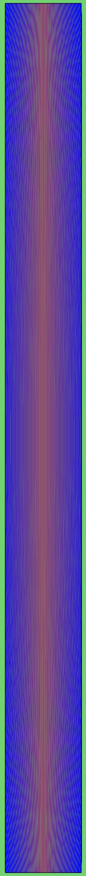
Speeding up:
•Increased temperature gradient
•Optimized heat transfer (convection)

•Better alternative: avoid (i.e. reduce object size)

Benefits of slow heat transfer:
•No thermal damage to interior in short high-temperature treatment of outer surfaces (e.g. „Baked Alaska“)

Diffusion as a challenge: Heat

Self-heating systems



Diffusion as a challenge: Heat

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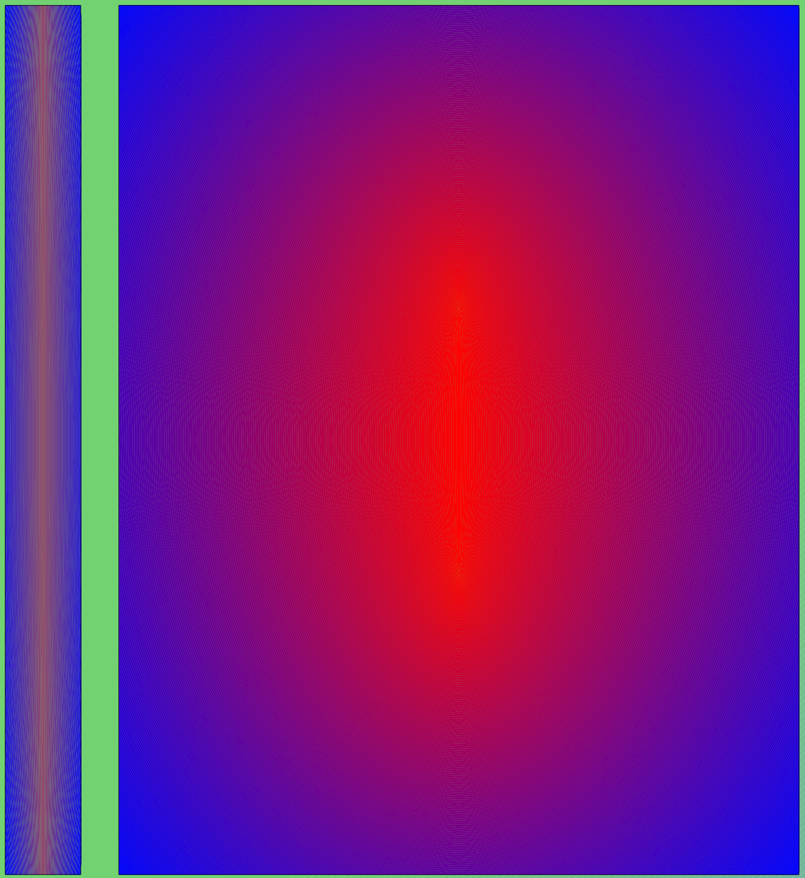
Self-heating systems



- Substantially higher temperatures in extended objects (e.g. over 80 °C in massive concrete structures vs. almost neglegible heating in slender structures)

Diffusion as a challenge: Heat

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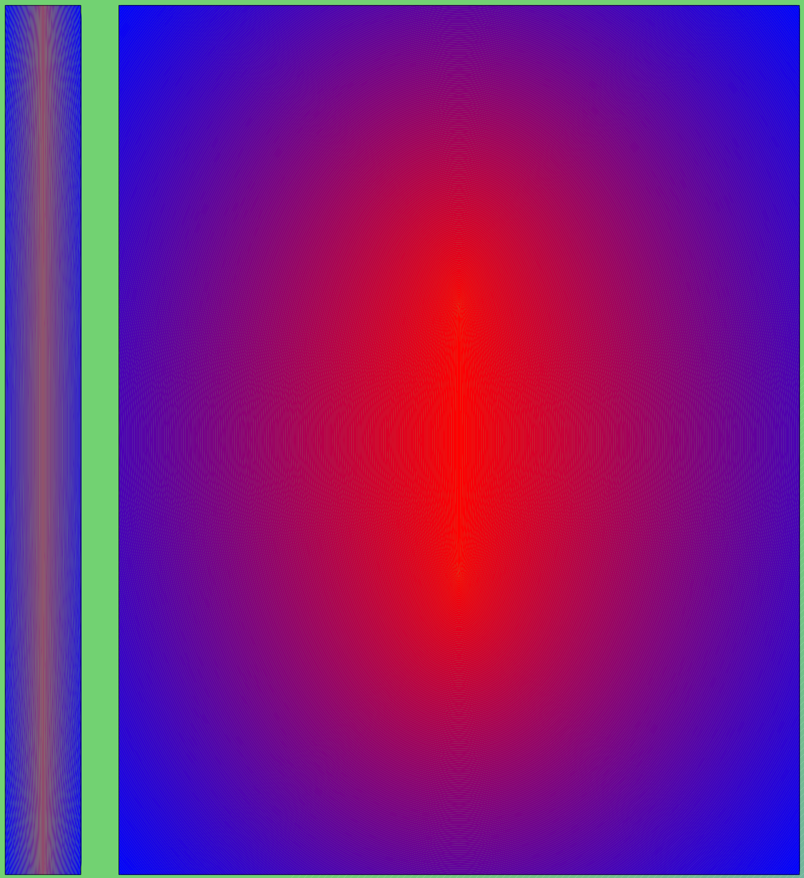
Self-heating systems



- Substantially higher temperatures in extended objects (e.g. over 80 °C in massive concrete structures vs. almost neglegible heating in slender structures)
- Especially problematic for reactions with positive temperature coefficient
  - Major danger in scale-up of reactions (power excursions!)
  - Countermeasures: keep S/V constant, increase stirring to achieve better heat exchange, active cooling

Diffusion as a challenge: Heat

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Heat-diffusion in buildings

Nordic

Alpine

Similar static heat conduction through walls

Low heat capacity

High heat capacity

Diffusion as a challenge: Heat

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Calderone Glacier @ Gran Sasso
25/08/07

Diffusion as a challenge reactants

Traditional tanks and reactors:

Large Péclet numbers

Exceptions:
- Heat exchangers
- Intraparticle processes

Diffusion as a challenge reactants

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Traditional tanks and reactors:

Large Péclet numbers

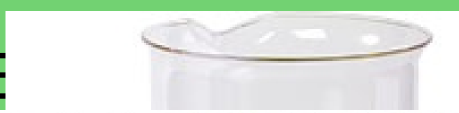
Active mixing processes needed

- In low viscosity systems: induce turbulence
  - Shorter length scales for diffusive mixing
  - Smaller **Pe**

Diffusion as a challenge reactants

Traditional tanks and reactors:

Large Péclet numbers



Active mixing processes needed

- In low viscosity systems: induce turbulence
  - Shorter length scales for diffusive mixing
  - Smaller $\mathbf{Pe}$
- High viscosity systems
  - Thorough mixing increasingly difficult
  - Typically lower D, too

Diffusion as a challenge reactants

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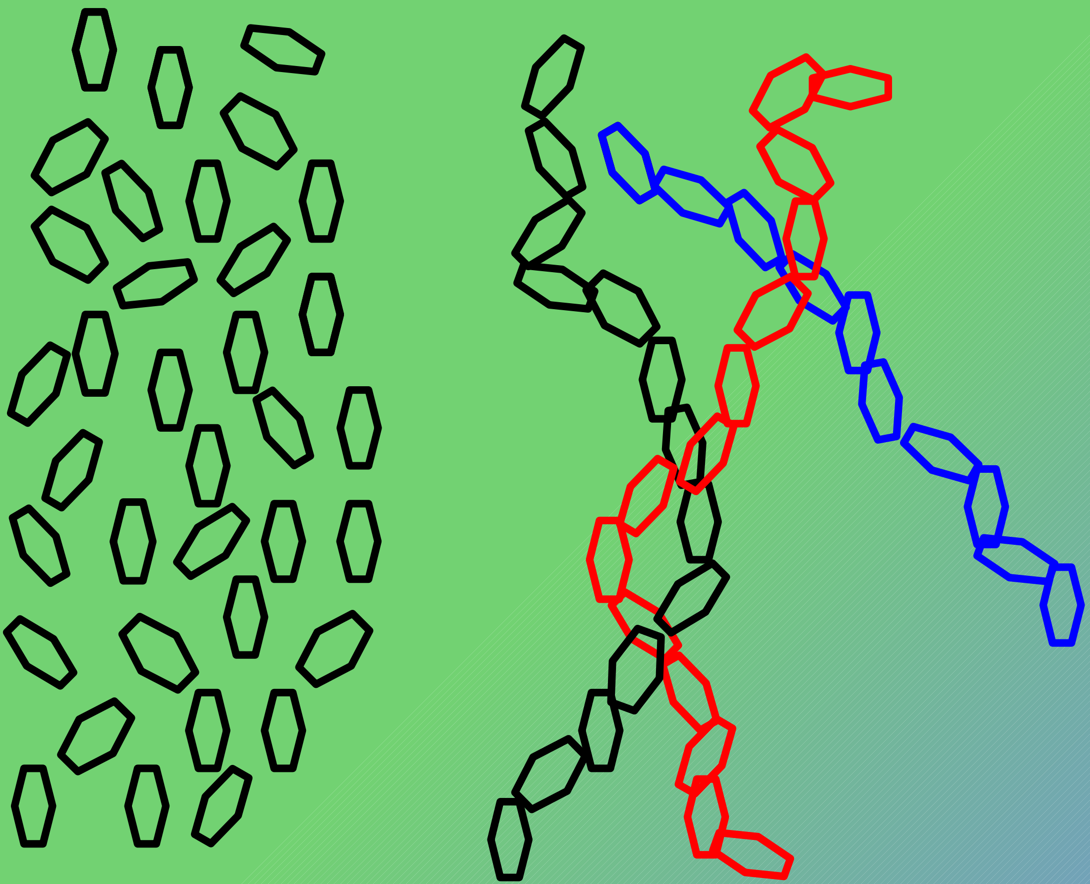
Polymerization reactions: especially strong increase in viscosity due to entanglement effects.



- Degree of polymerization
- <u>Polymer concentration (solution processes)</u>

  yield!
- Branching and crosslinks

Diffusion as a challenge reactants

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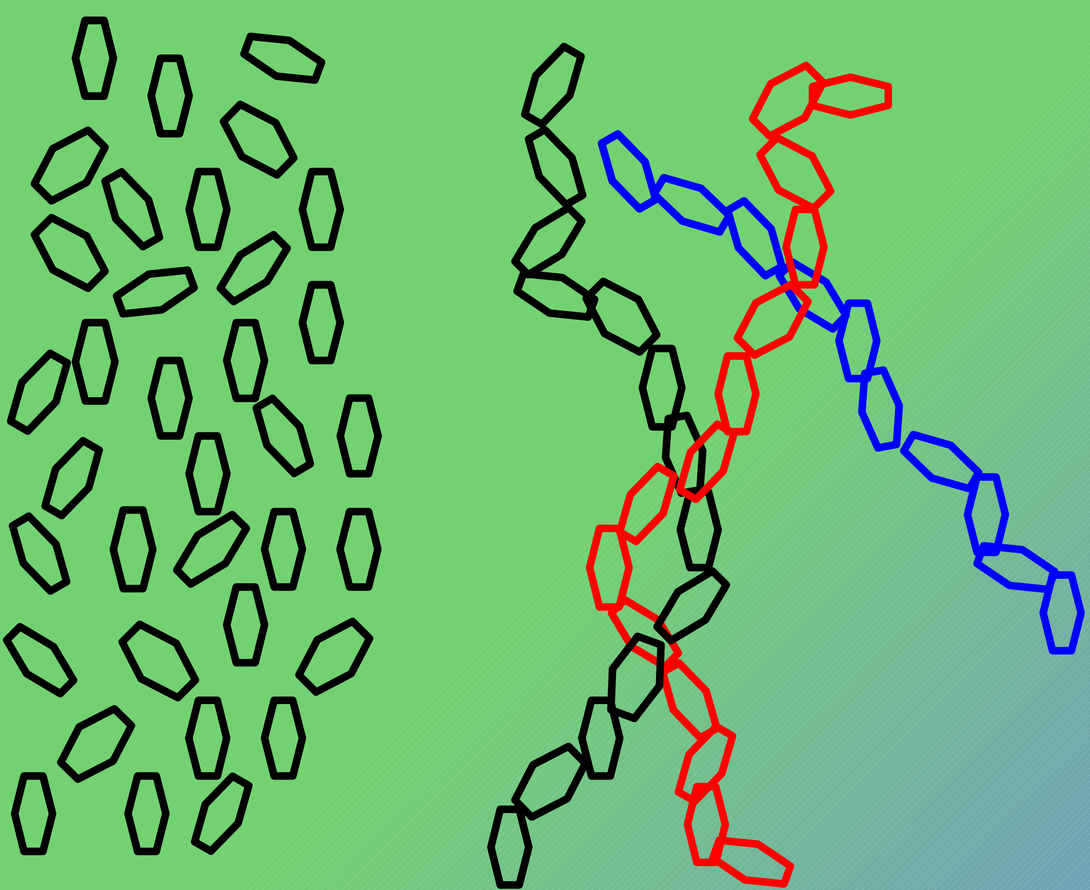
Polymerization reactions: especially strong increase in viscosity due to entanglement effects.



- Degree of polymerization
- <u>Polymer concentration (solution processes)</u>
  yield!
- Branching and crosslinks

- Residual monomers
- Plasticizers

Diffusion as a challenge reactants

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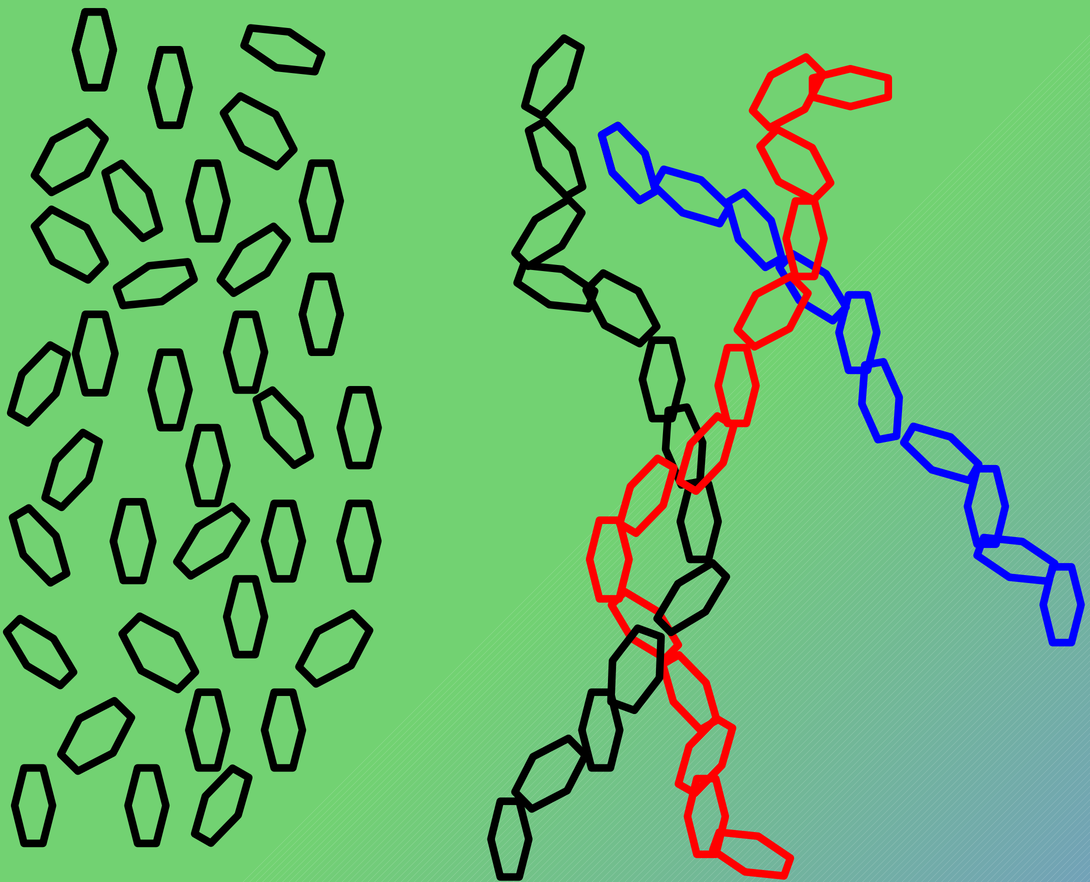
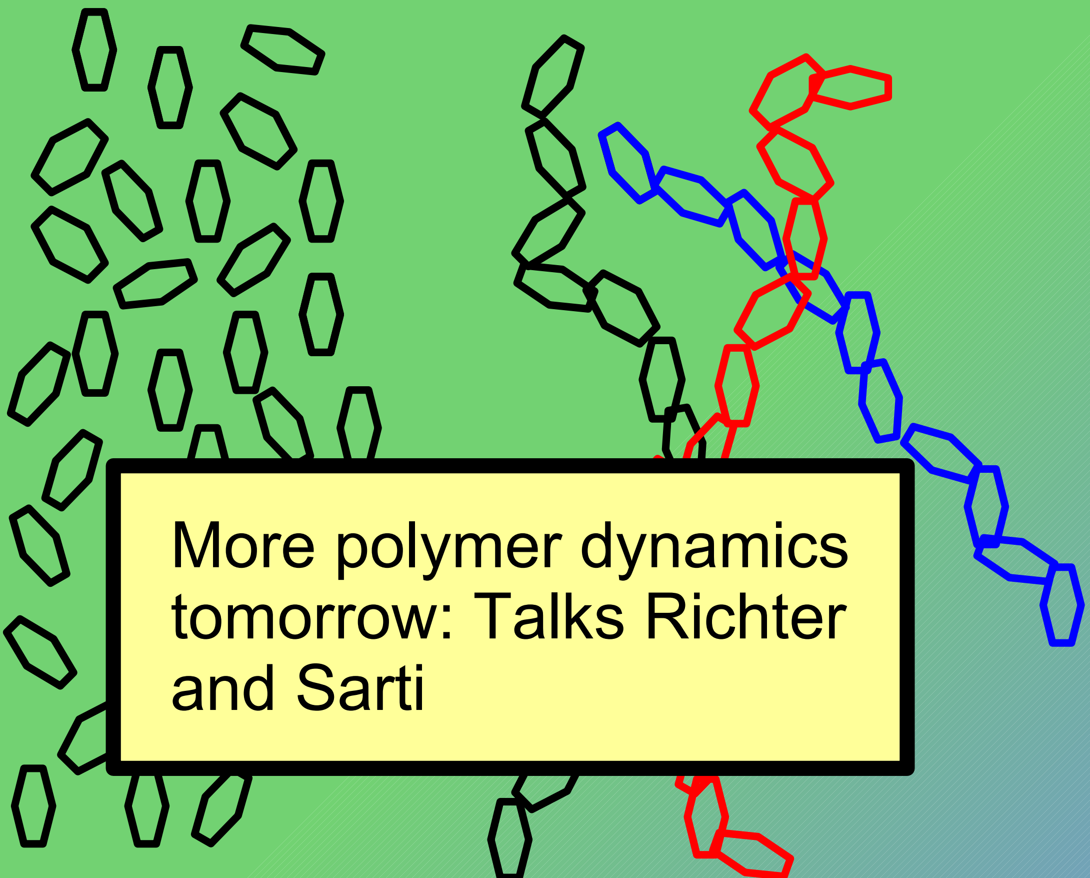


- Degree of polymerization
- Polymer concentration (solution processes)
  yield!
- Branching and crosslinks

- Temperature
  heating energy!
  decomposition!
- Residual monomers
- Plasticizers

Diffusion as a challenge reactants

Polymerization reactions: especially strong increase in viscosity due to entanglement effects.



More polymer dynamics tomorrow: Talks Richter and Sarti

- Degree of polymerization
- <u>Polymer concentration (solution processes)</u>
  yield!
- Branching and crosslinks

- <u>Temperature</u>
  heating energy!
  decomposition!
- Residual monomers
- Plasticizers

Diffusion as a challenge reactants

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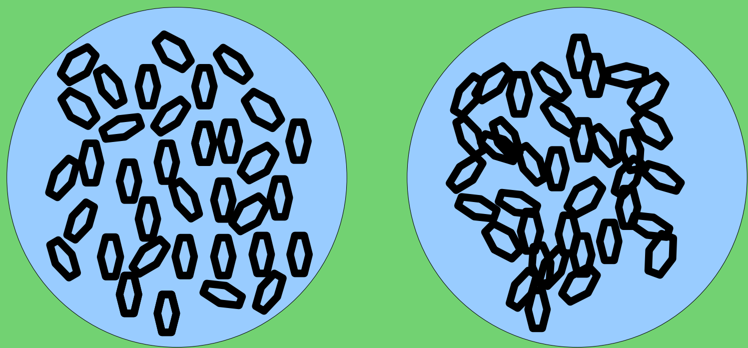
Alternative approach to polymerizations: emulsion polymerization



- Especially attractive for production of cross-linked polymers
- Diffusive transport only at length scale of droplets or micelles
- Low-viscosity convection in continous liquid phase

Diffusion as a challenge reactants

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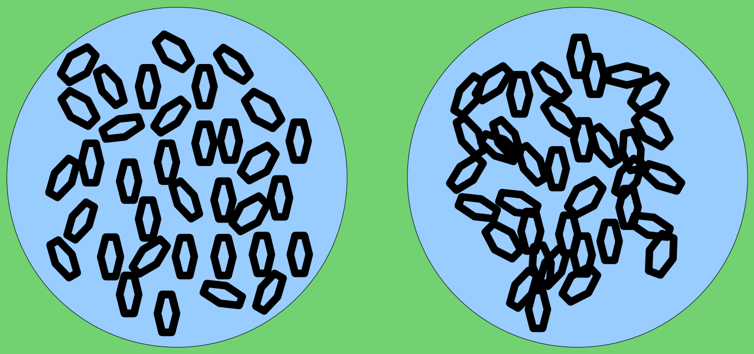
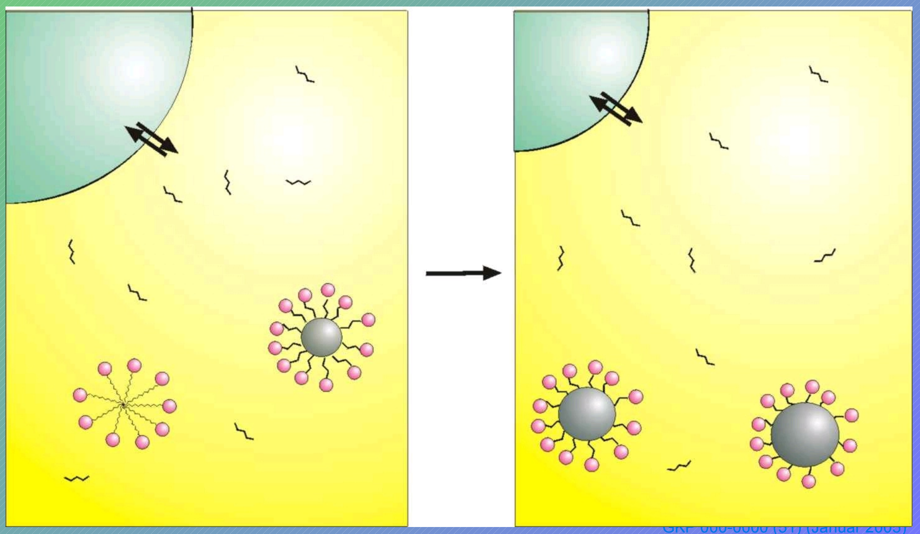
Alternative approach to polymerizations: emulsion polymerization



- Especially attractive for production of cross-linked polymers
- Diffusive transport only at length scale of droplets or micelles
- Low-viscosity convection in continous liquid phase

- Different modes of operation depending on distribution of monomers and starters
- Surfactant material needed
- Most typical case: oil-in water emulsions
- Monodisperse particles from ordered micellar phases



Diffusion as a challenge reactants

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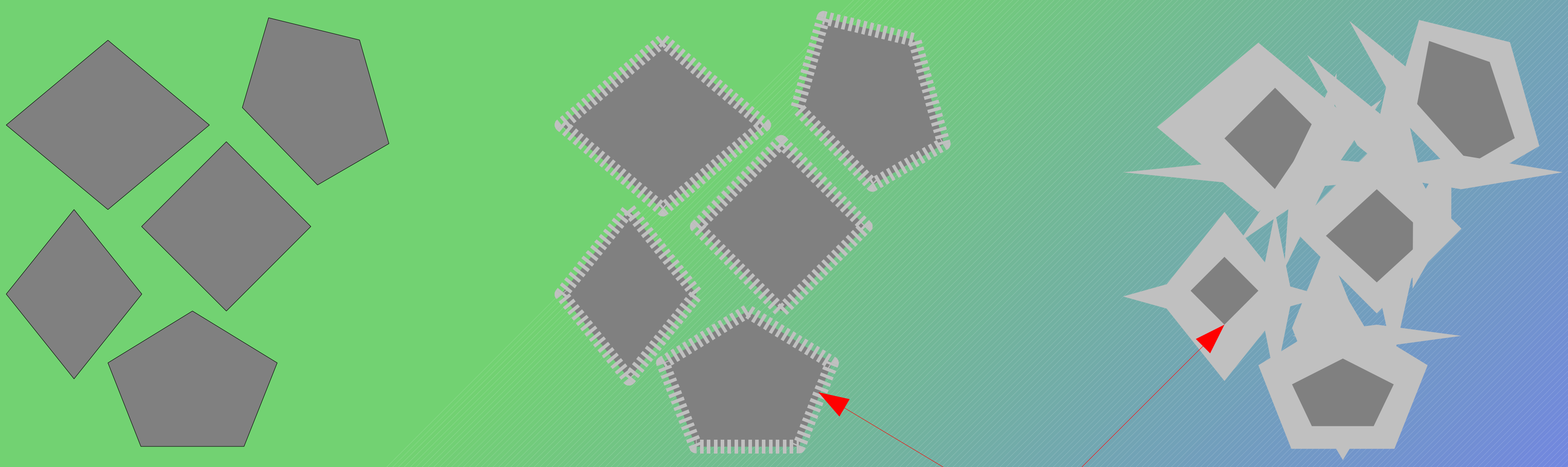
Cement hydration:
Dissolution of suspended clinker grains

Reprecipitation of CSH phases



Dissolution of unreacted cement clinker increasingly impeded by CSH diffusion barrier

- Delayed hydration
- poor use of clinker

Diffusion as a challenge reactants

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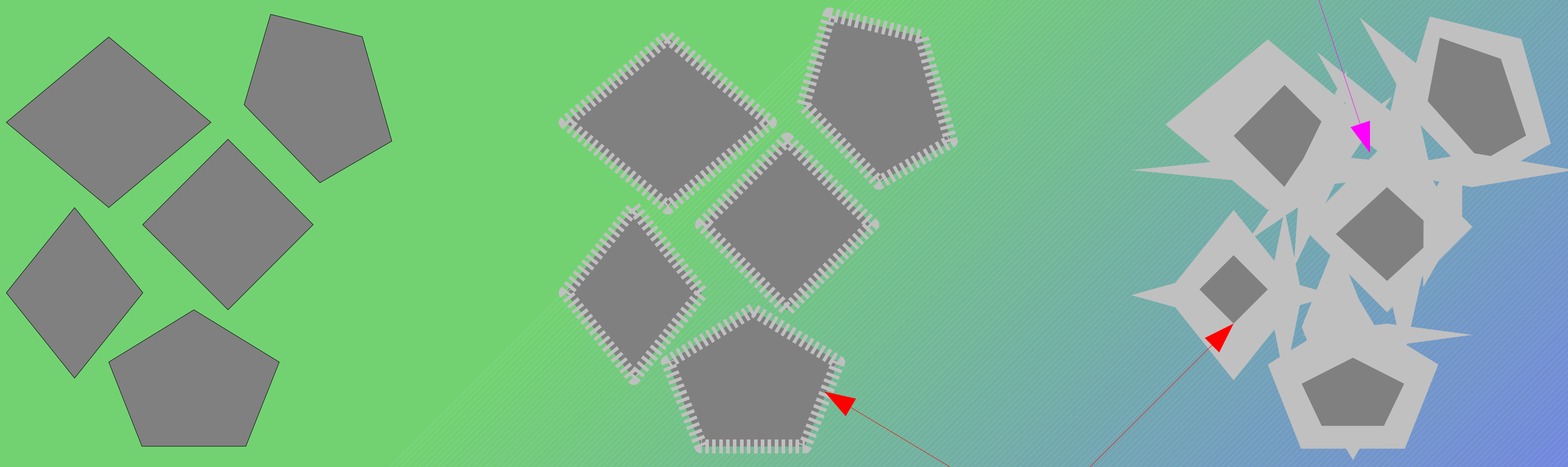
Cement hydration:
Dissolution of suspended clinker grains

Poster C03 Bordallo et al. :
water in CSH phases

Repreciptation of CSH phases



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Diffusion as a challenge reactants

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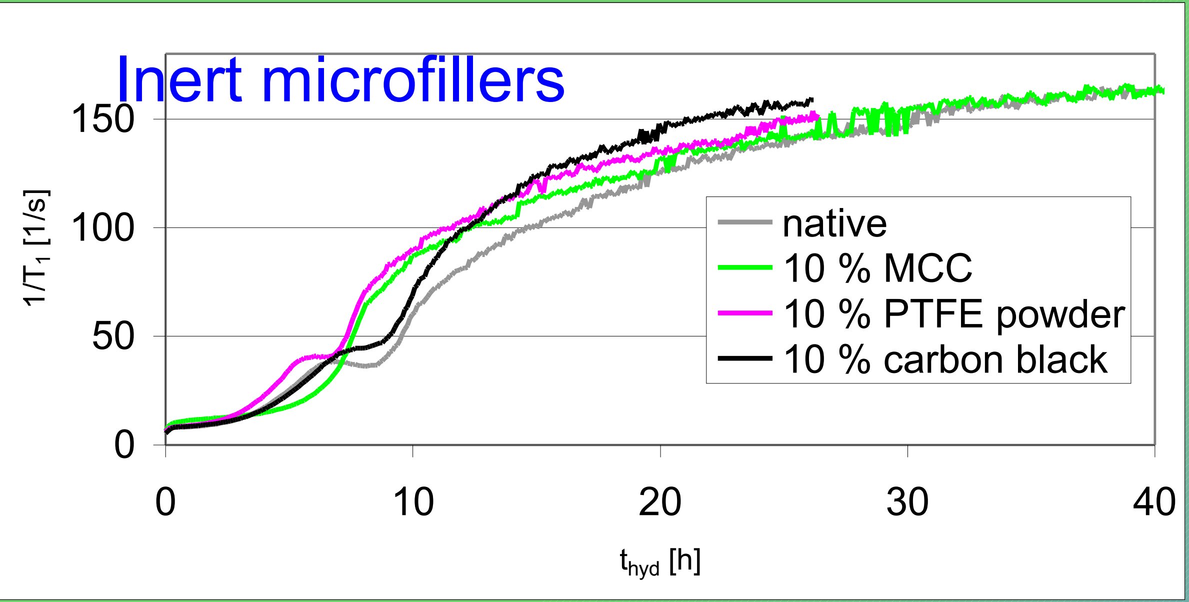
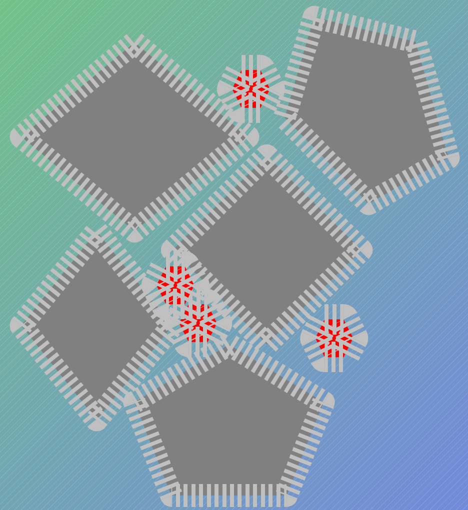
Enhanced hydration in the presence of microfillers



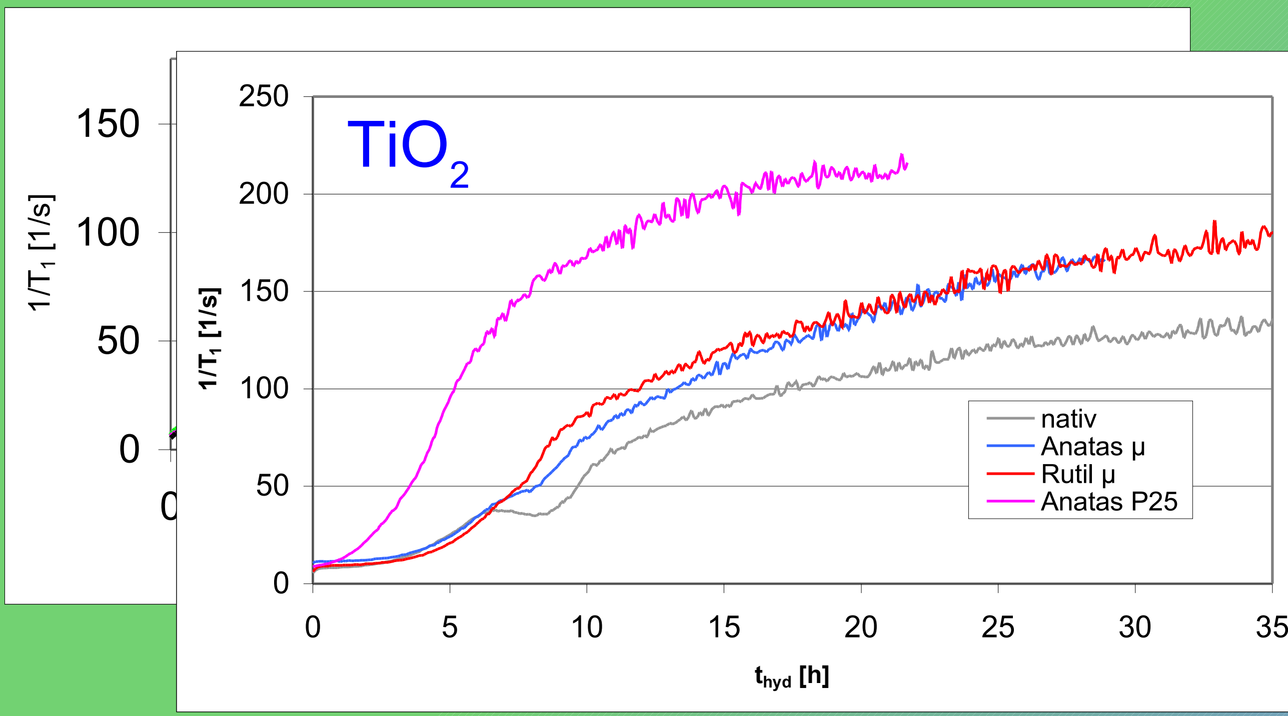


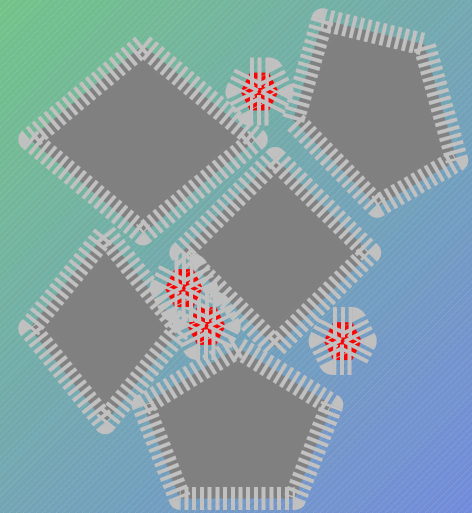
Cement hydration kinetics studied by TD-NMR

$1/T_1$ essentially proportional to S/V inside cement stone matrix

Diffusion as a challenge reactants

Enhanced hydration in the presence of microfillers





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Diffusion as a challenge reactants

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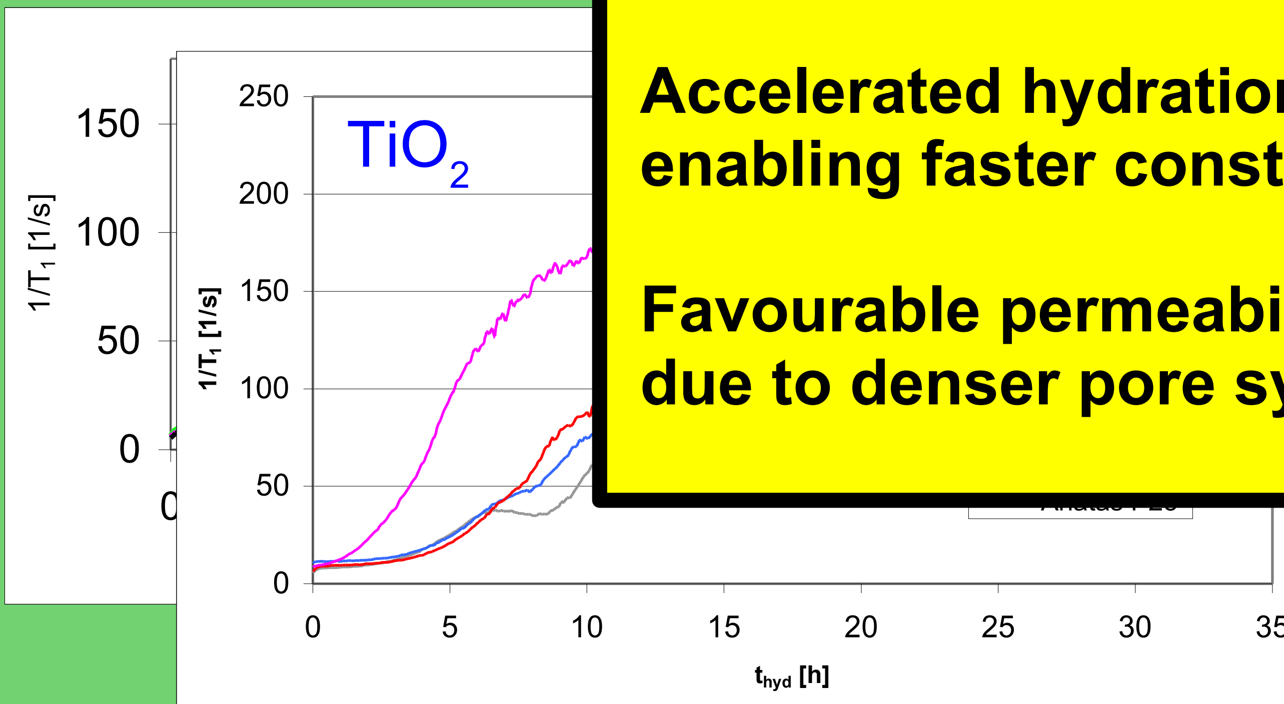


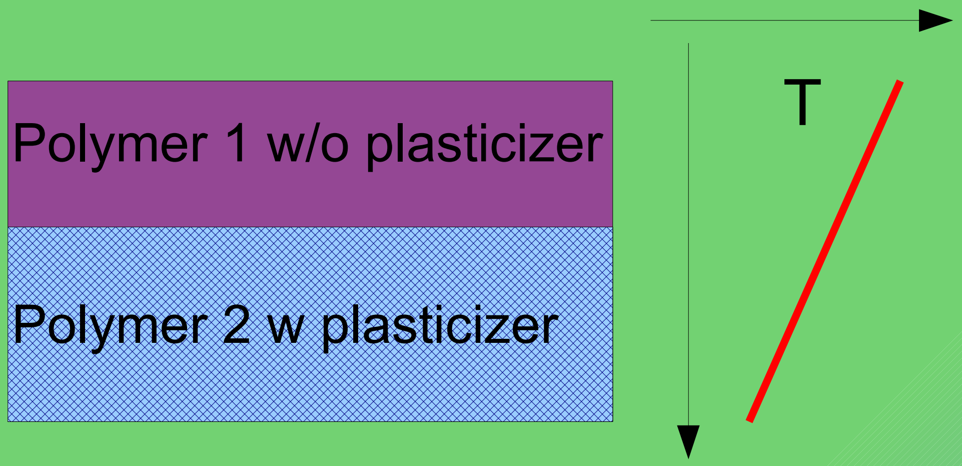
Accelerated hydration desirable for enabling faster construction.

Favourable permeability properties due to denser pore system.

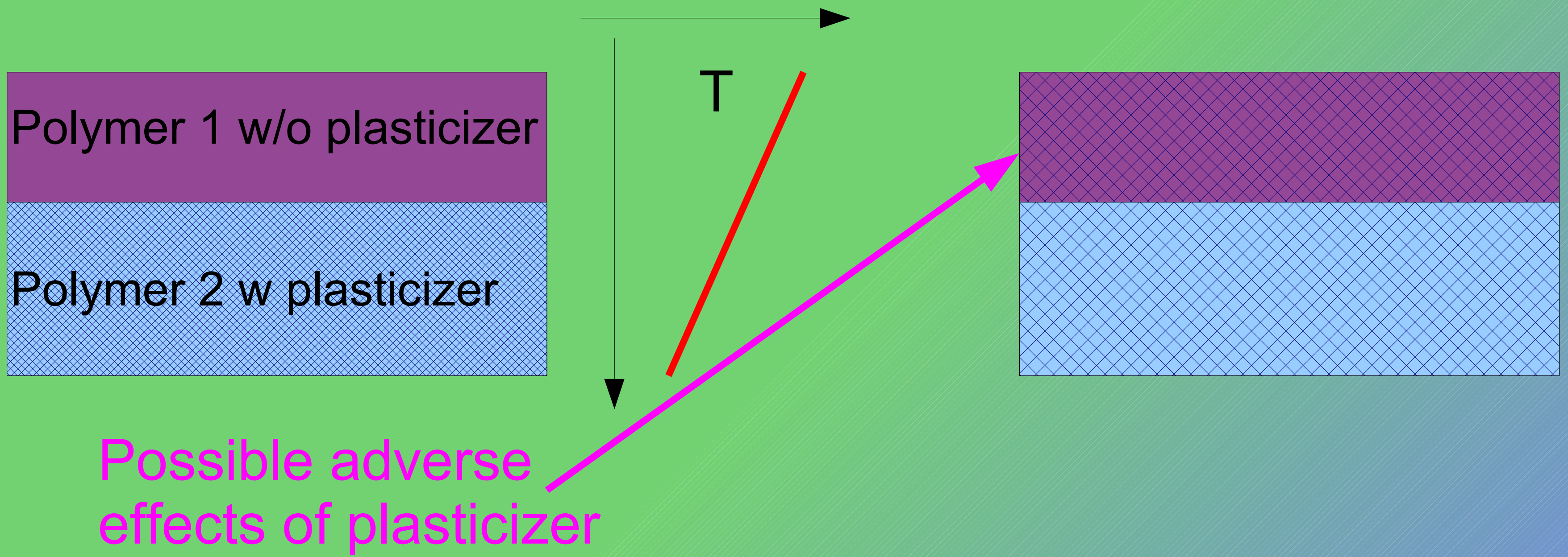
Cement hydration kinetics studied by TD-NMR

$1/T_1$ essentially proportional to S/V inside cement stone matrix

Diffusion as a challenge composite products



Diffusion as a challenge composite products



Diffusion as a challenge composite products

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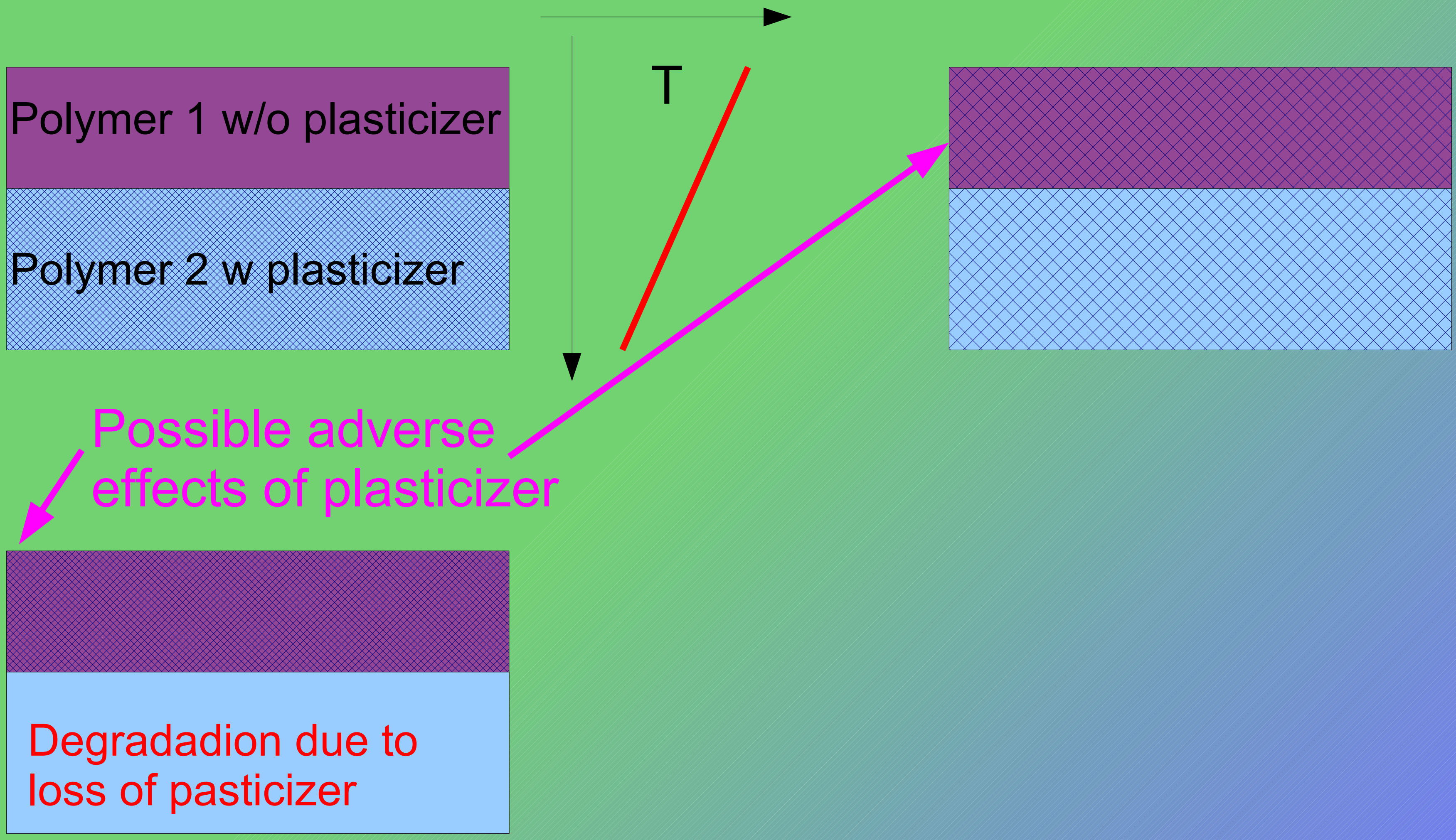

Diffusion as a challenge composite products

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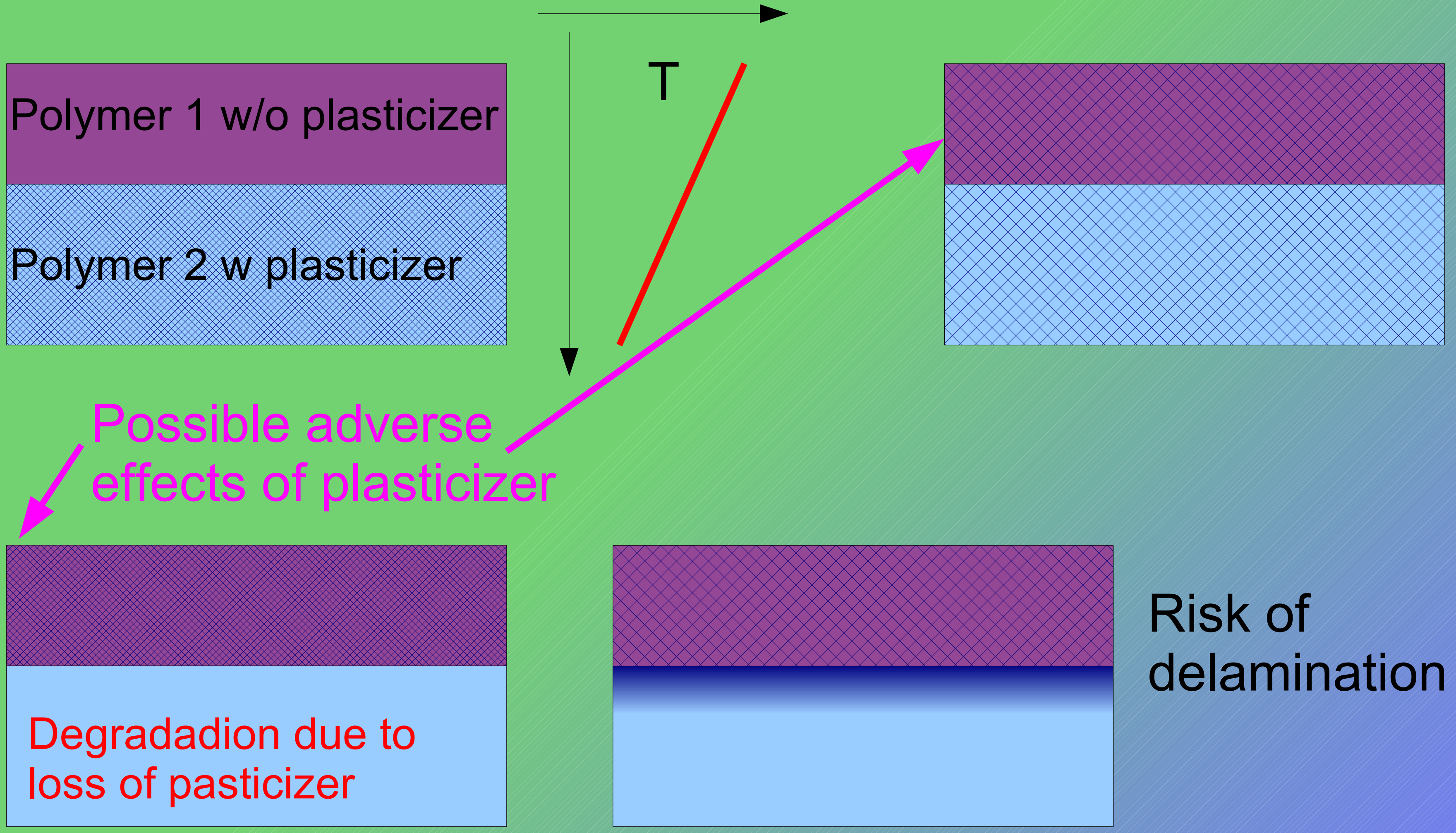

Diffusion as a challenge composite products

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Polymer 1

Polymer 2

Possi
effect

Parameters affecting diffusion effects in composite materials

- Distribution coefficient between two layers
- Miscibility (possibly temperature effects)
- Diffusion coefficient

Measures against diffusion

- Reduction of diffusion coefficient
- Introduction of barriers

Degradadion due to loss of pasticizer

Diffusion as a challenge composite products

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Polymer 1

Polymer 2

Possi
effect

Parameters affecting diffusion effects in composite materials

- Distribution coefficient between two layers
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- Diffusion coefficient

Measures against diffusion

- Reduction of diffusion coefficient
- Introduction of barriers

Degradadion due to loss of pasticizer

Polymer 1 w/o plasticizer

Polymer 2 w plasticizer

Diffusion as a challenge food

- Natural diffusion barriers
  - Outer skins: essential self-protection systems of organisms against loss of moisture and oxydation

Diffusion as a challenge food

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- Natural diffusion barriers
  - Outer skins: essential self-protection systems of organisms against loss of moisture and oxydation

Shelf-life

Diffusion as a challenge food

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- Natural diffusion barriers
  - Outer skins: essential self-protection systems of organisms against loss of moisture and oxydation
  - Internal barriers: helping to maintain local concentration gradients

Shelf-life

Diffusion as a challenge food

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- Natural diffusion barriers
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Shelf-life

- Inside „homogeneous“ tissues:
  - Almost free diffusion (water and/or vapour phase) in extracellular media
  - Possibly even faster transport pathways due to capillary effects
  - Barrier action of cell walls much weaker than outer barriers

Diffusion as a challenge food

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Shelf-life

Drying

Diffusion as a challenge food

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  - Barrier action of cell walls much weaker than outer barriers

Processing and spicing

marinated and pickled foods

- In absence of outer barriers: 1 cm/day
- Whole fruit with intact skin (e.g. olives): months

Diffusion as a challenge food

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Processing and spicing

marinated and pickled foods
- In absence of outer barriers: 1 cm/day
- Whole fruit with intact skin (e.g. olives): months

Mechanical or osmotic disruption of barriers before frying

Diffusion as a challenge food composites

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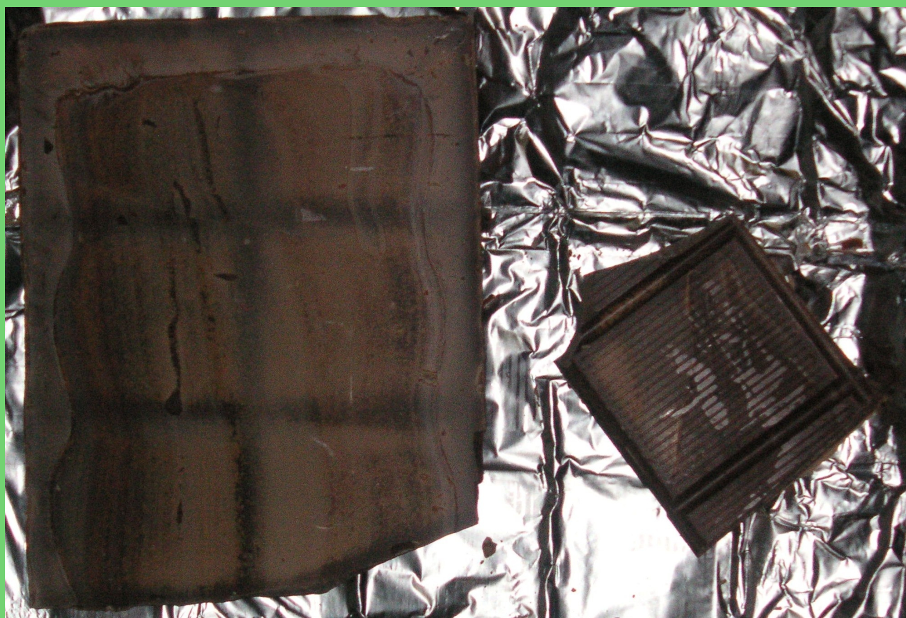
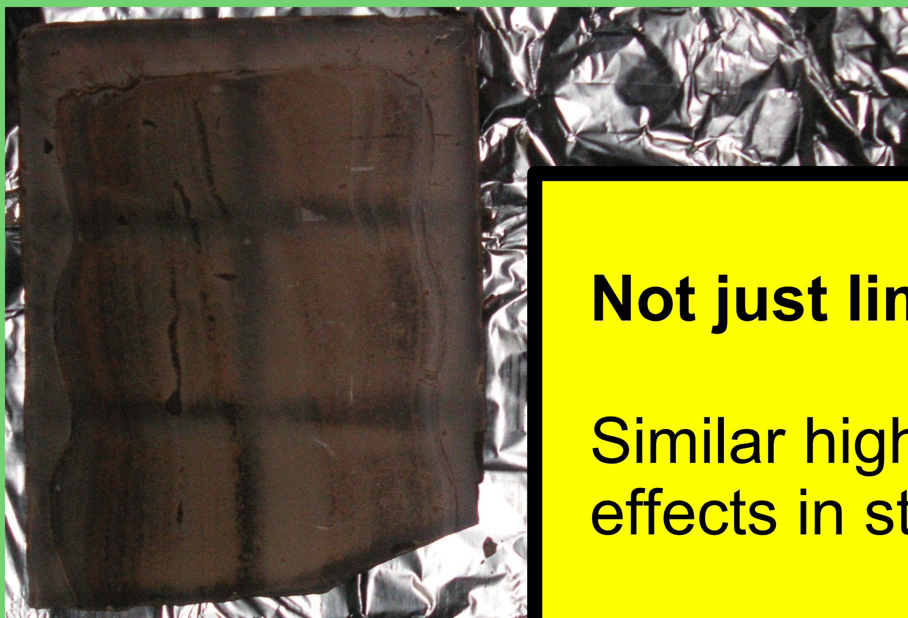


(Organic) chocolate after a few weeks with occasional heating episodes up to 30 °C (i.e. in a kitchen without air conditioning)

Macroscale demixing of solid and liquid fat components and diffusion to the surface

Similar effect in a Bacio with internal (macroscopic) fat-fat interfaces

Diffusion as a challenge food composites



(Organic) chocolate after
a few weeks with occasional
s up to 30 °C
without air

ixing of solid
mponents and
urface

a Bacio with
internal (macroscopic) fat-fat
interfaces

Not just limited to food:

Similar high-temperature effects in steel.

Posters B1, B2 Evteev et al.

Diffusion as a challenge food composites

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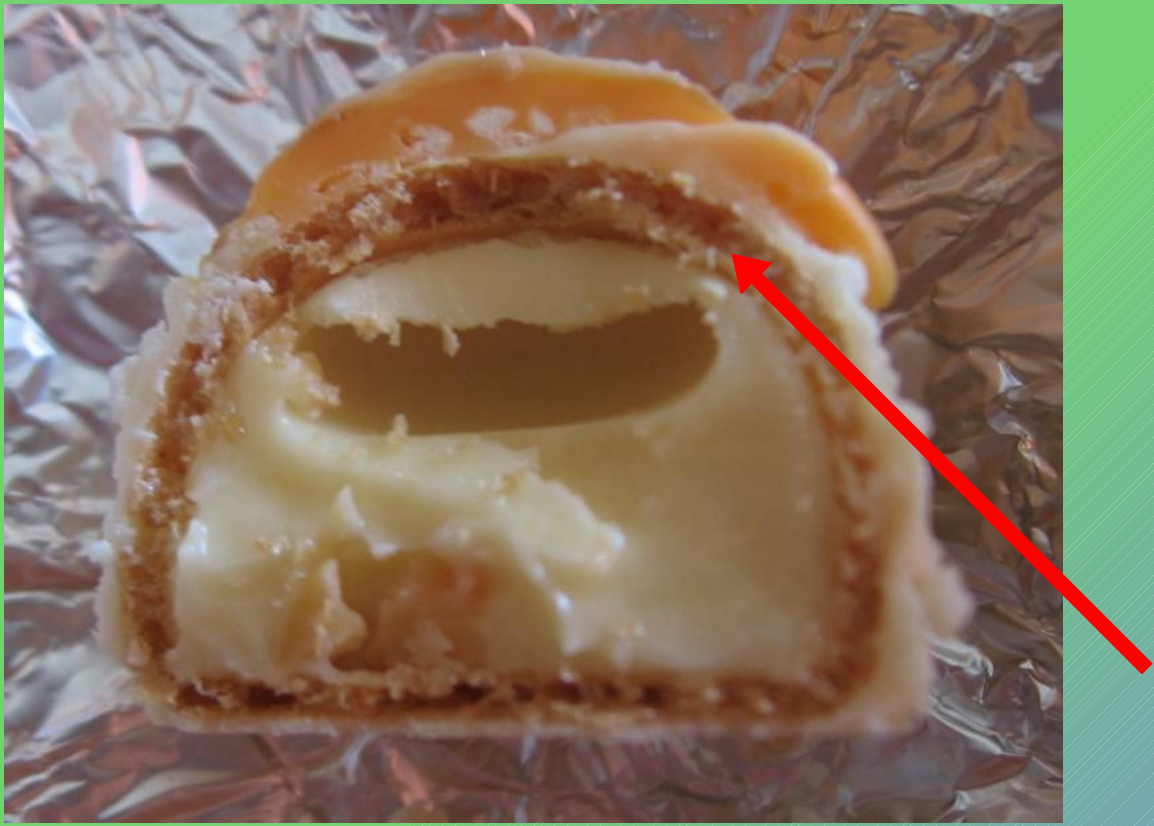

A sweets manu-facturers' crunchy trick to control diffusive transport between different fat phases

Insert a hydrophilic cracknel
capillary barrier between the two fatty layers

Diffusion as a friend: controlled release

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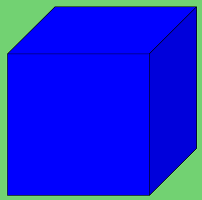
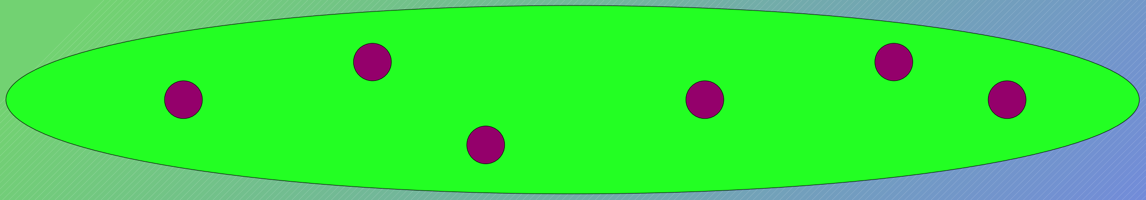


Active agent

Substrate Target



Diffusion as a friend: controlled release

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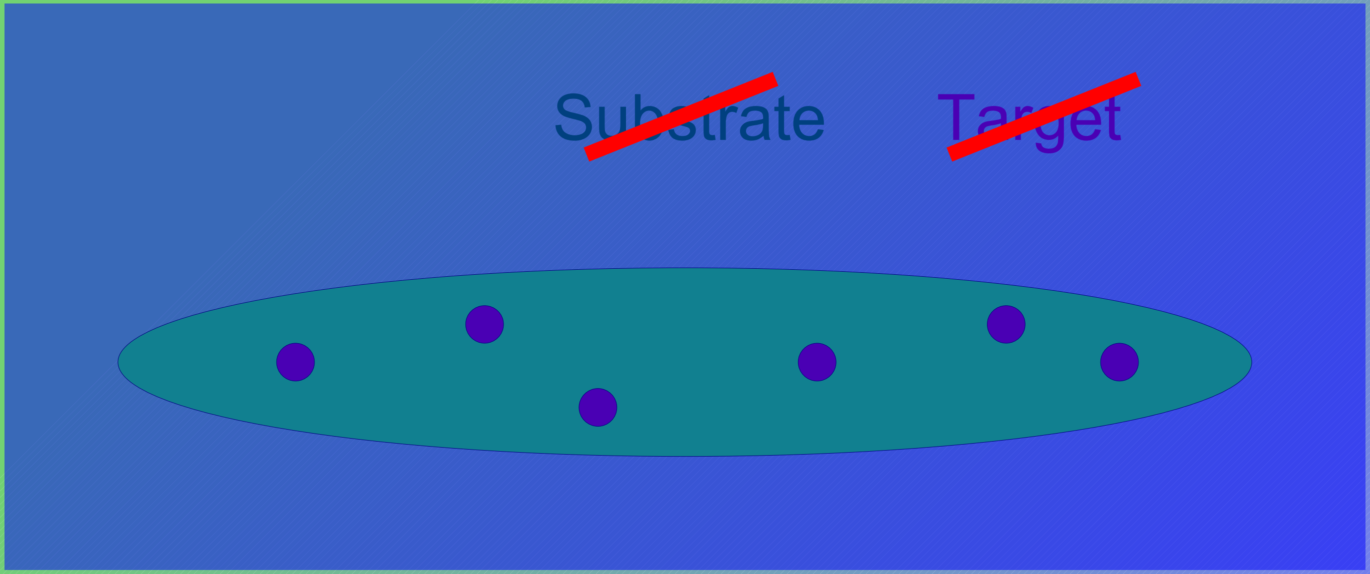
Active agent dissolved in high concentration

- Concentration difficult to maintain (e.g. washout, degradation)
- Side effects



Diffusion as a friend: controlled release

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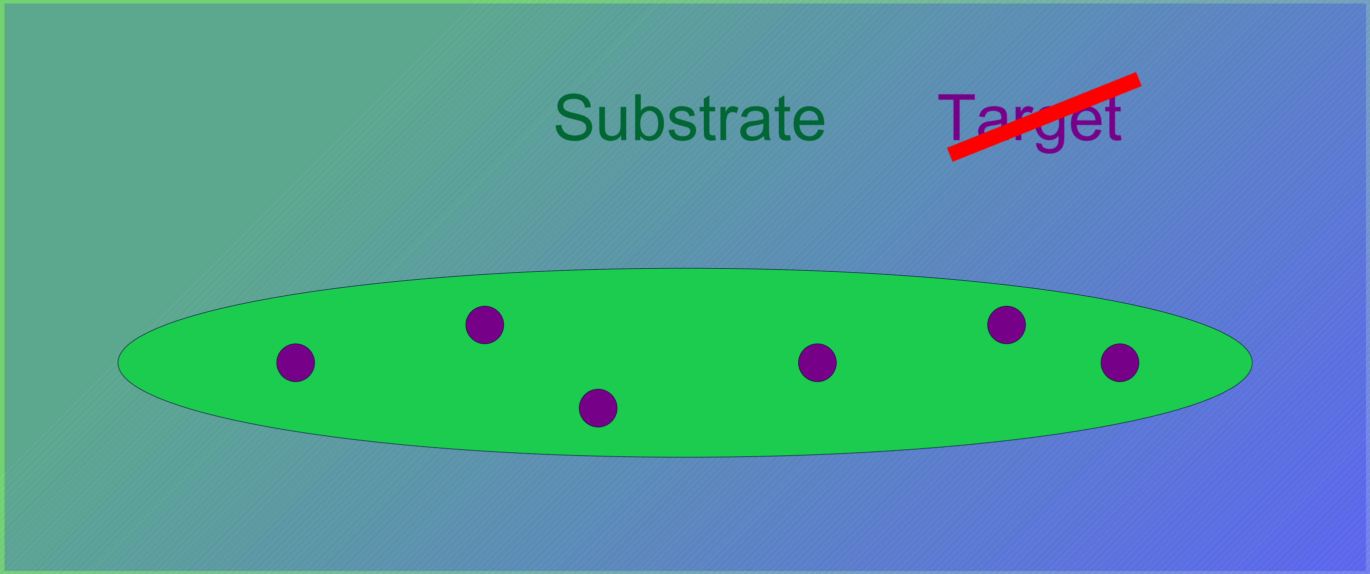
Active agent dissolved in low concentration
- Concentration difficult to maintain (e.g. washout, degradation)
- Less side effects



Diffusion as a friend: controlled release

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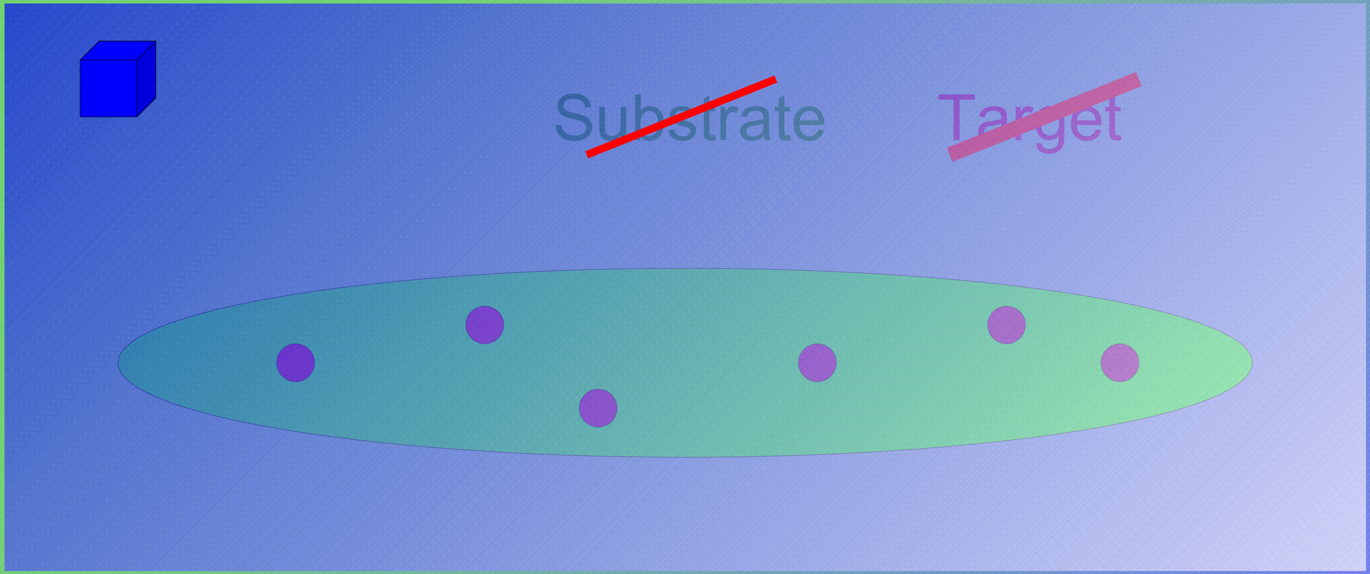
Constant supply of agent for dissolution:

- Desired effect: maintainance of a low and effective agent concentration for a long time



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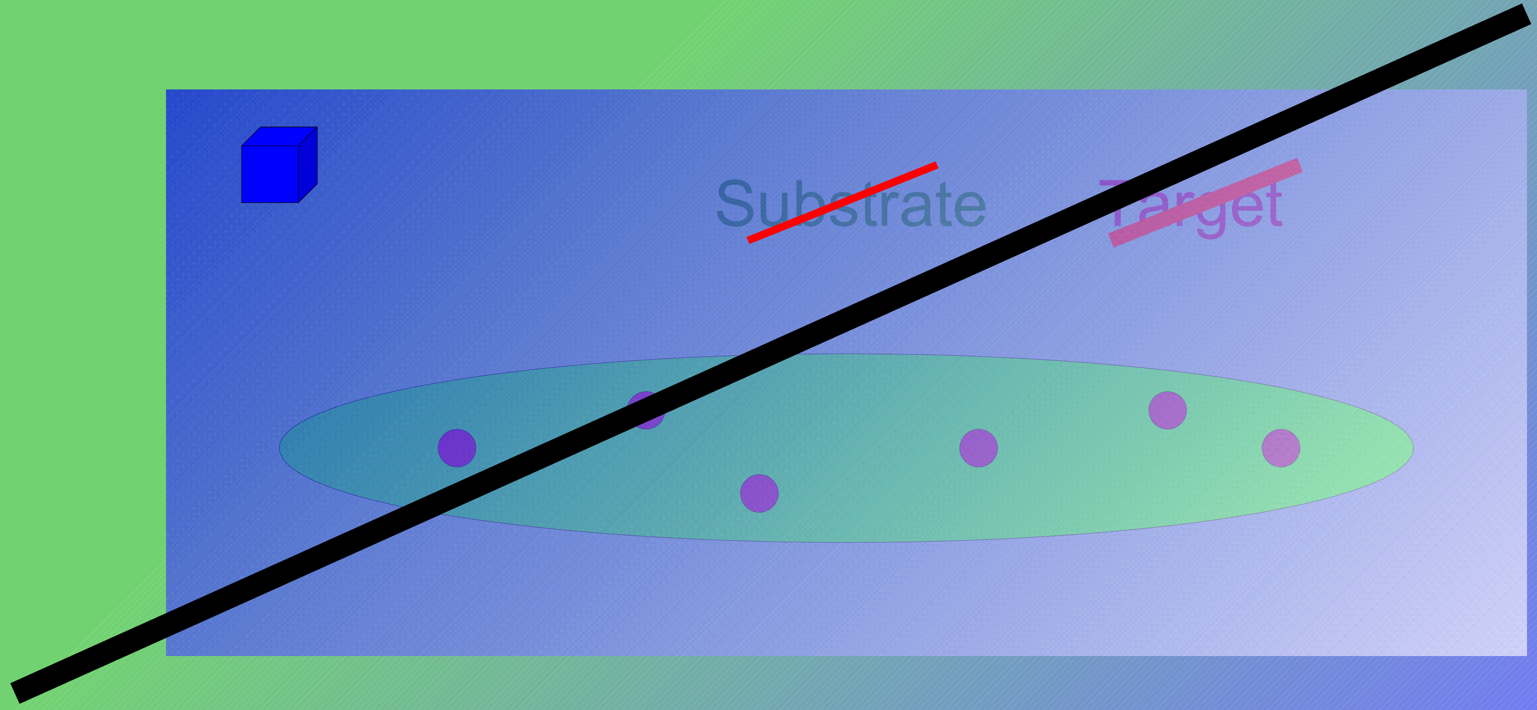

Diffusion as a friend: controlled release

Competence in Physics key to your success

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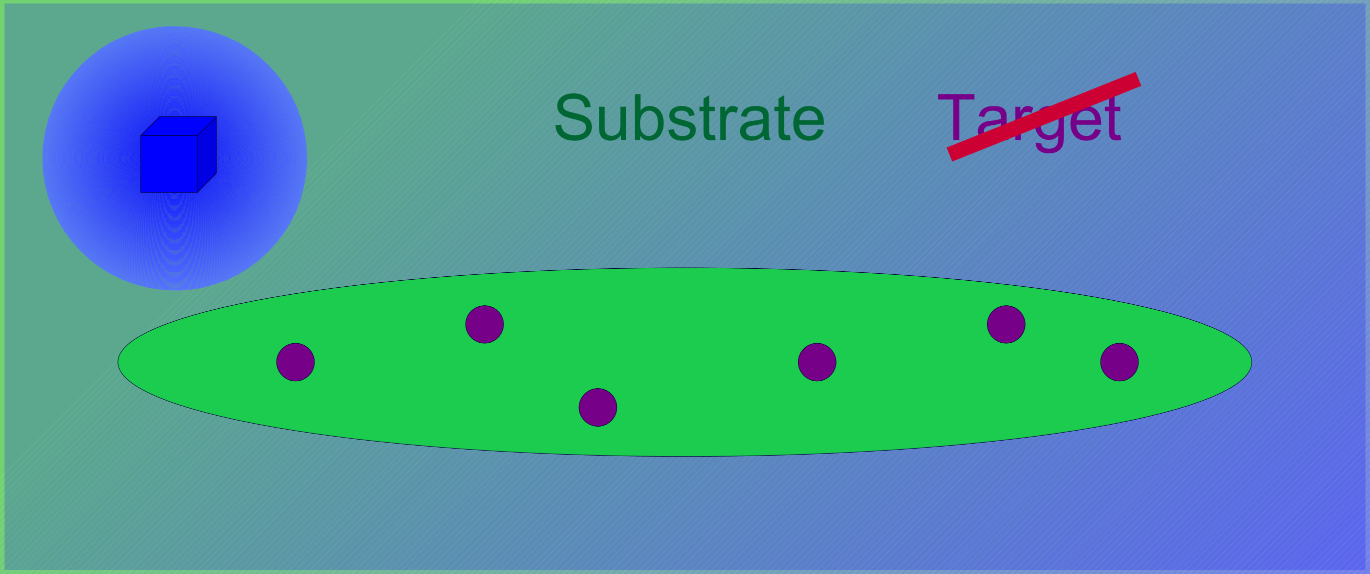


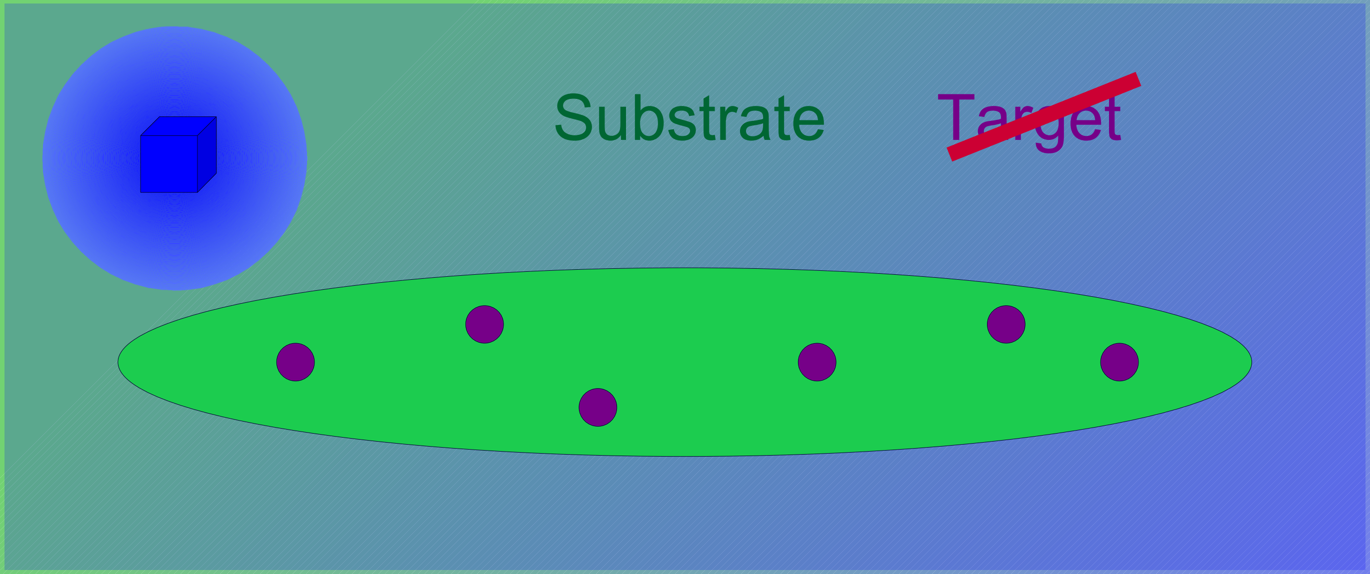
Diffusion as a friend: controlled release

Constant supply of agent for dissolution:

- Desired effect: maintainance of a low and effective agent concentration for a long time

Remaining challenges:

- Time profile of release
- Delayed onset of action
- Combination of several agents



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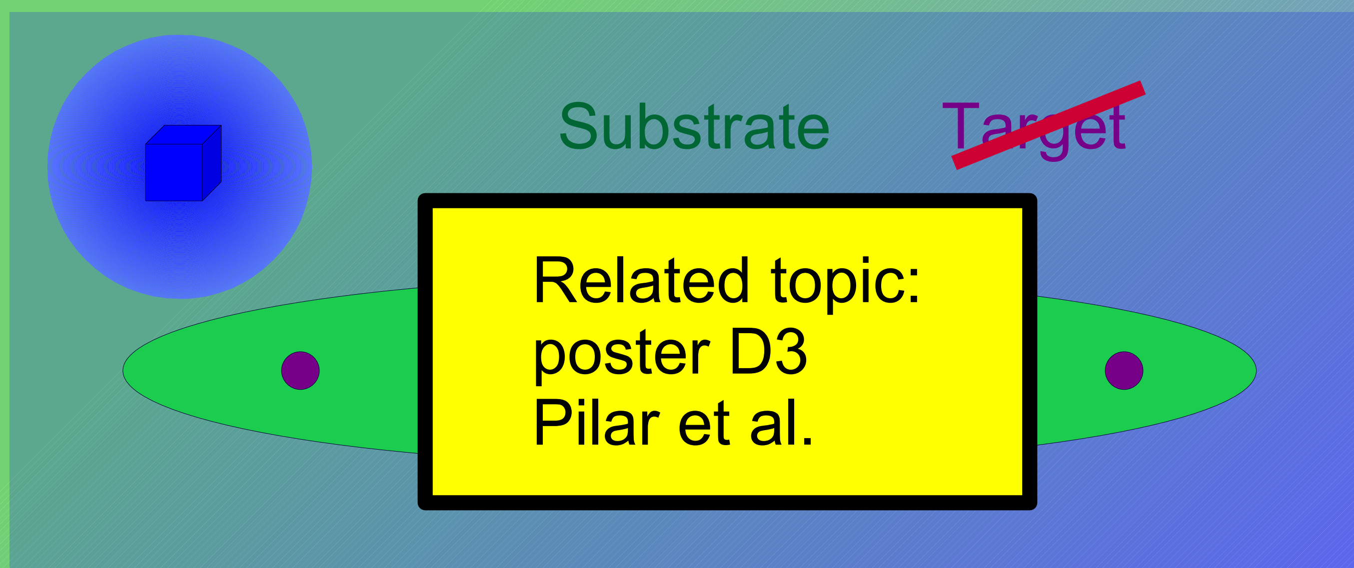

Going micro and nano: approaching the apparent dwarf

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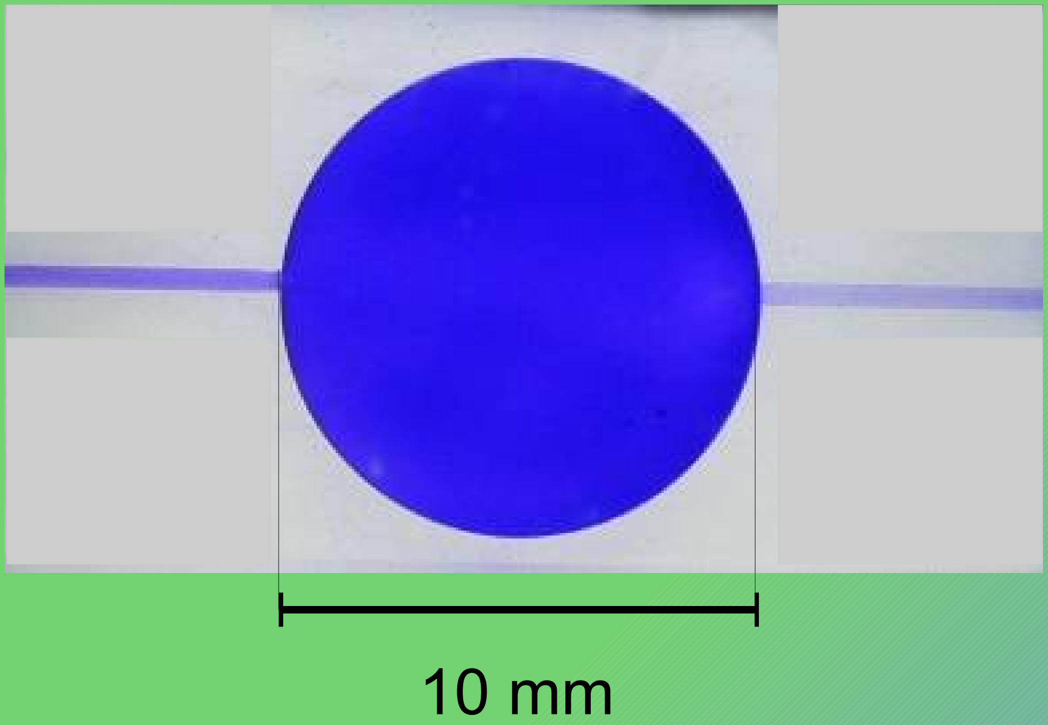
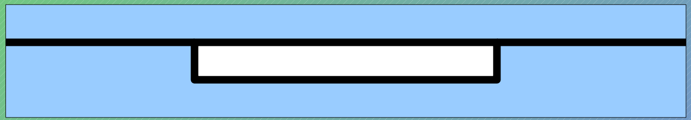


Washing out a blue colour tracer (C.I. Basic Violet 3) from a circular flat cell



Going micro and nano: approaching the apparent dwarf

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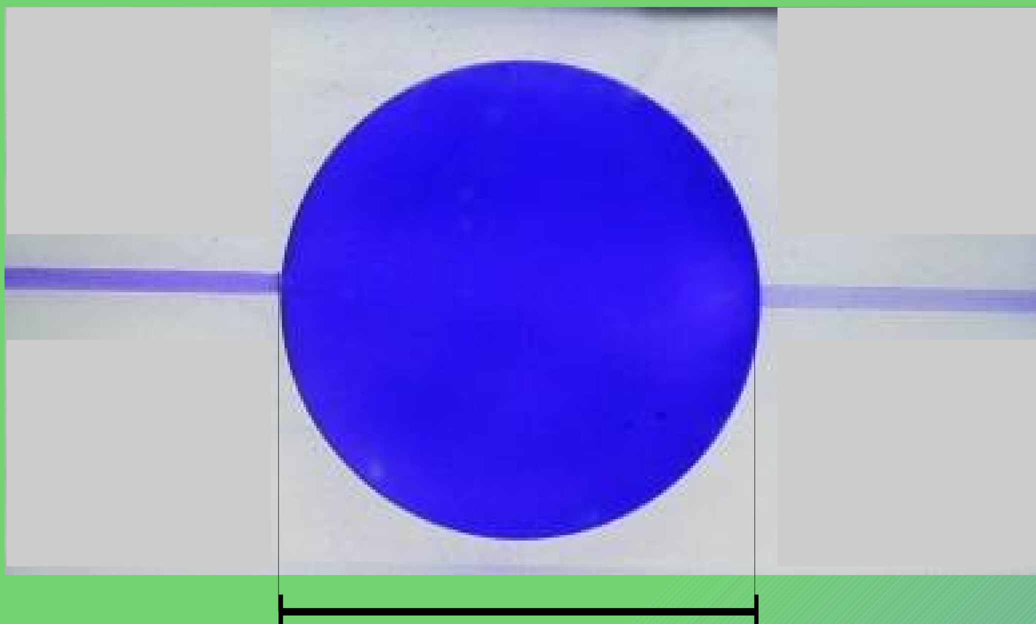
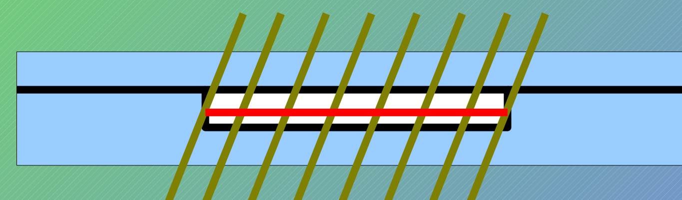


10 mm

Washing out a blue colour tracer (C.I. Basic Violet 3) from a circular flat cell



•Context: Interplay between diffusion and relaxation in thin excited slices

(A. Gädke and N.N., *Diffusion Fundamentals* **3** 38.1-38.12)

Going micro and nano: approaching the apparent dwarf

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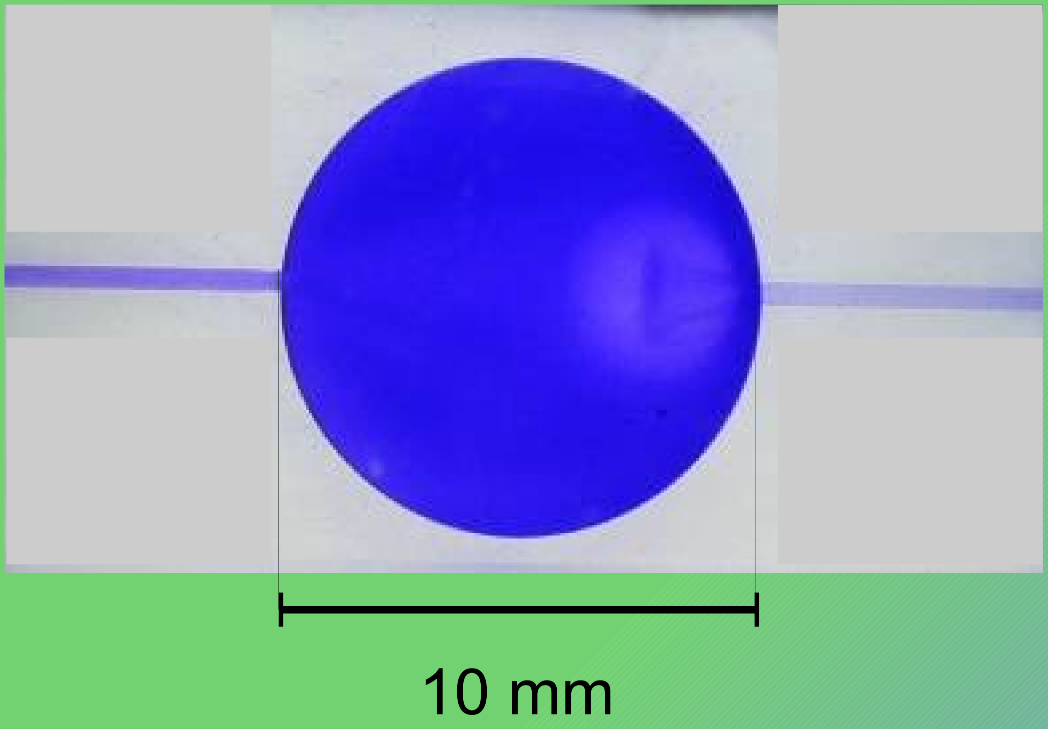

After 4.5 s of 10 ml/min water flow.

Going micro and nano: approaching the apparent dwarf

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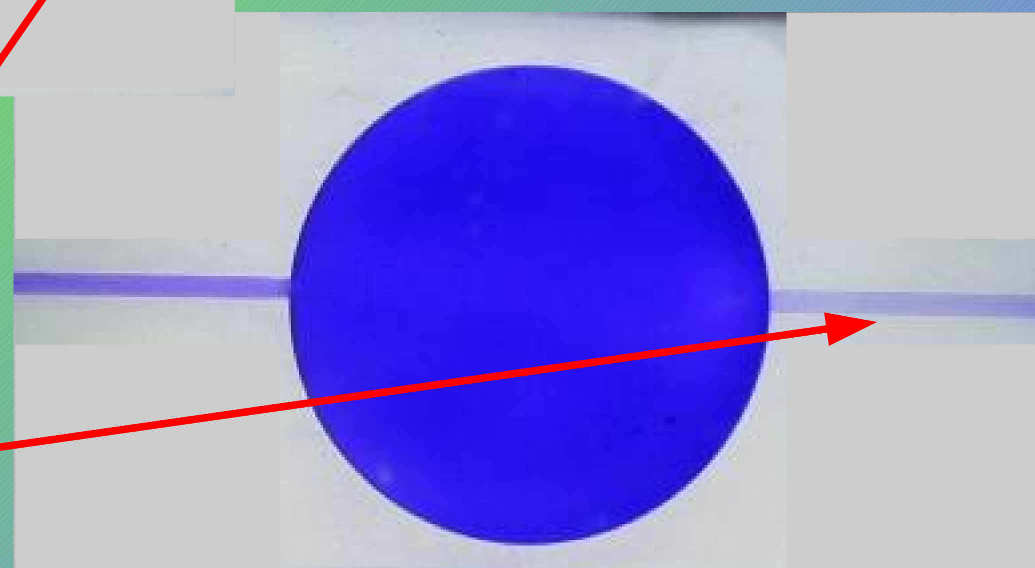
10 mm

After 4.5 s of 10 ml/min water flow.



Almost no notable decolouring of feed line

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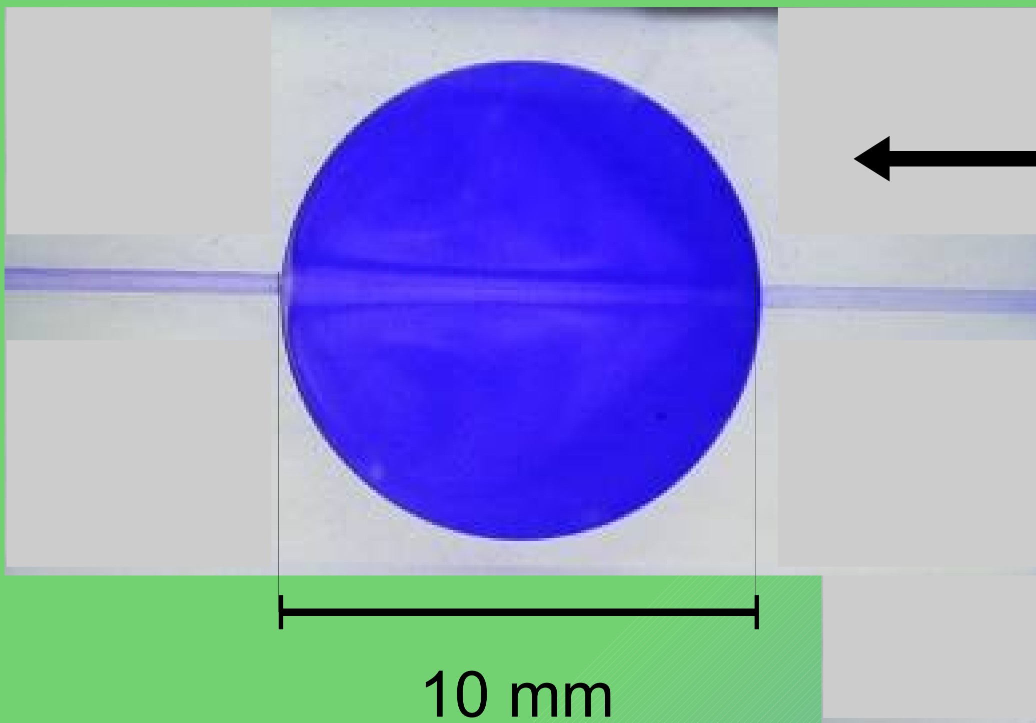
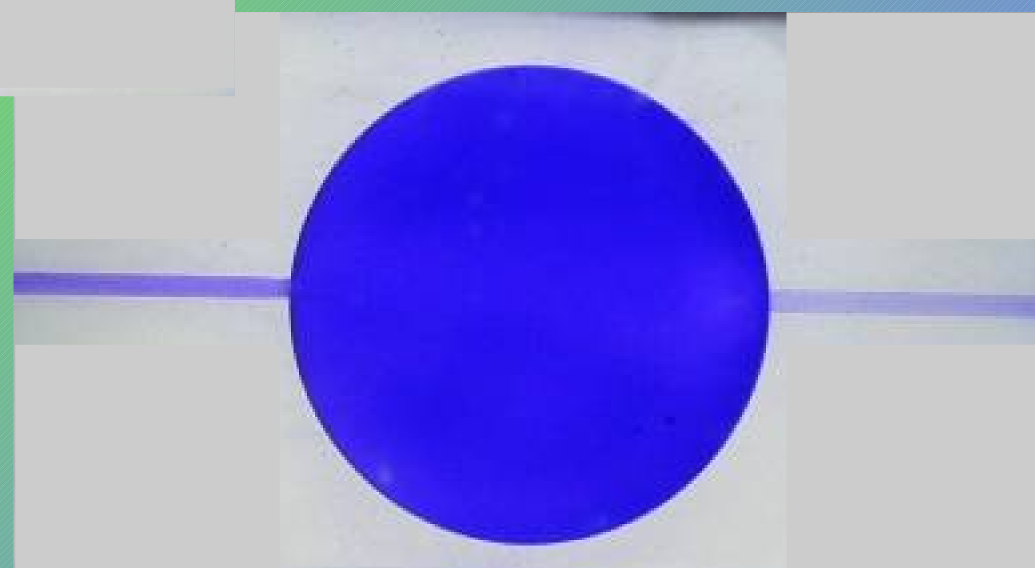


After 9 s of 10 ml/min water flow.



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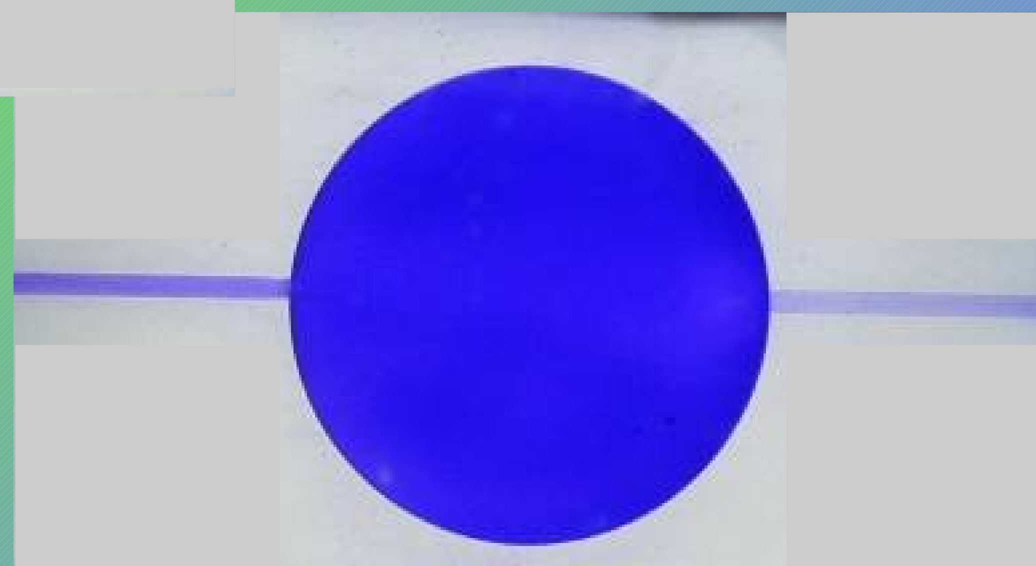
10 mm

After 13.5 s of 10 ml/min water flow.



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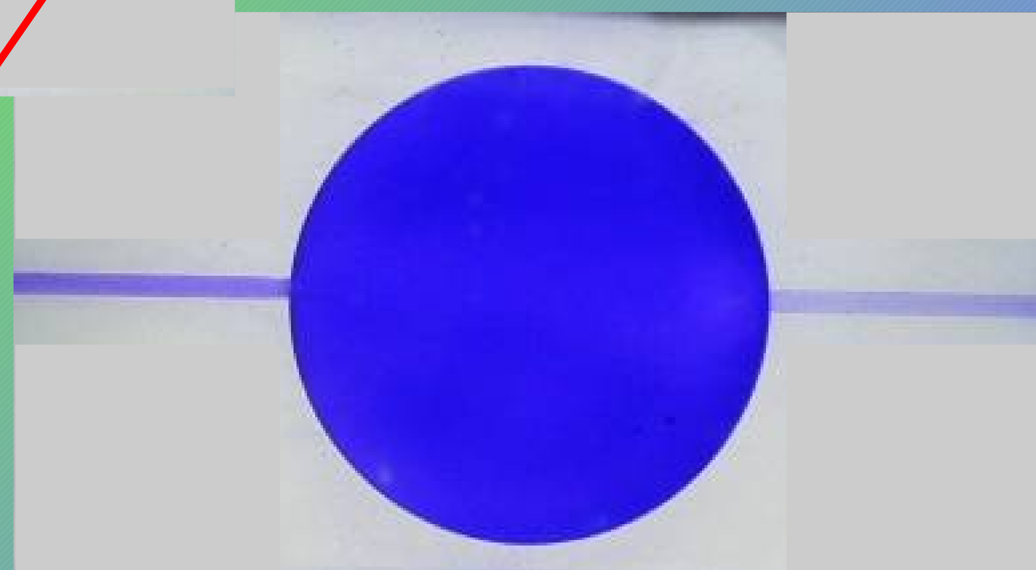
After 18 s of 10 ml/min water flow.

10 mm

Almost complete decolouring of feed line



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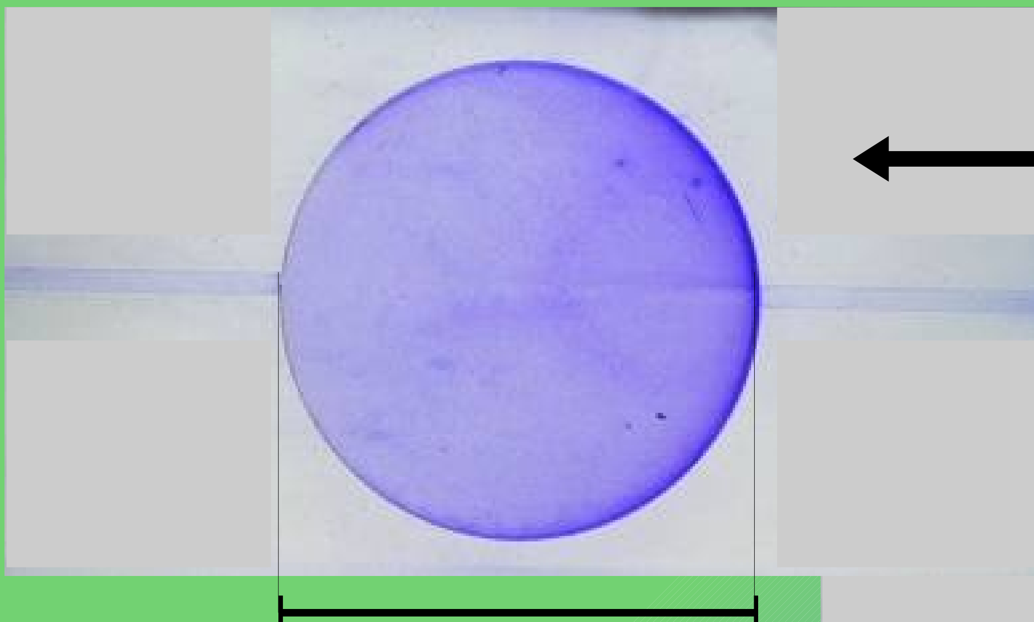
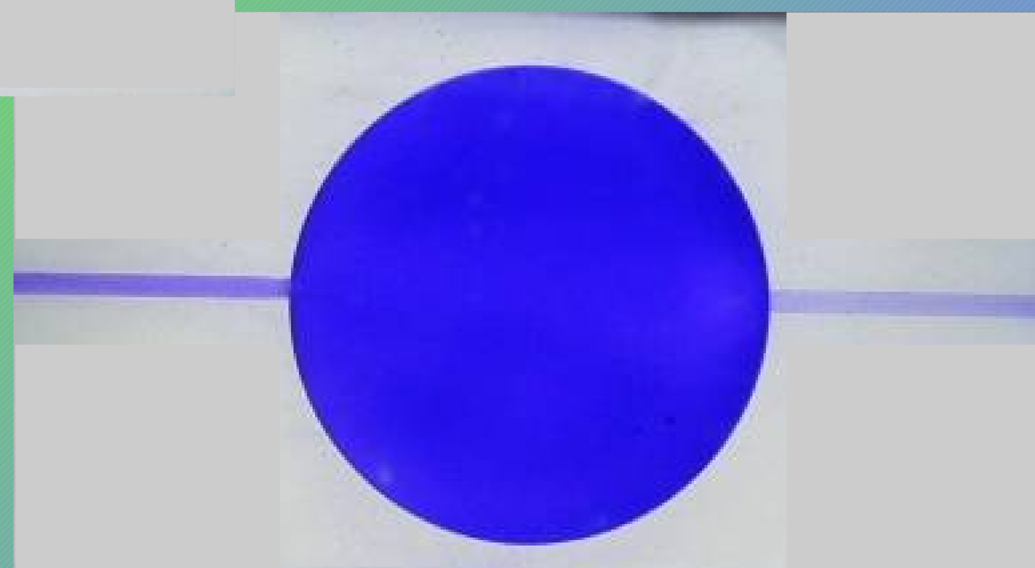


10 mm

After 22.5 s of 10 ml/min water flow.



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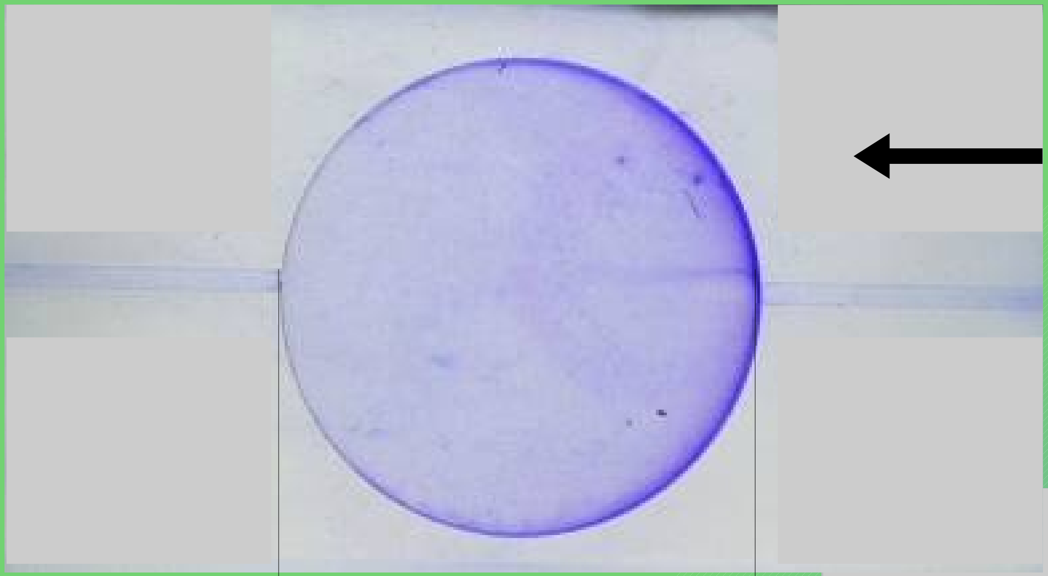
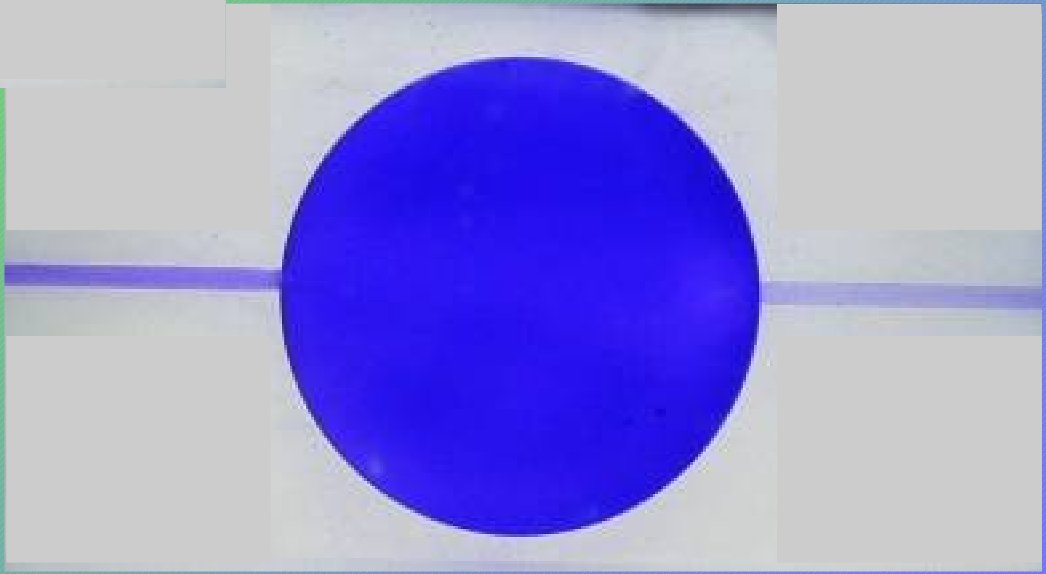


10 mm

After 27 s of 10 ml/min water flow.



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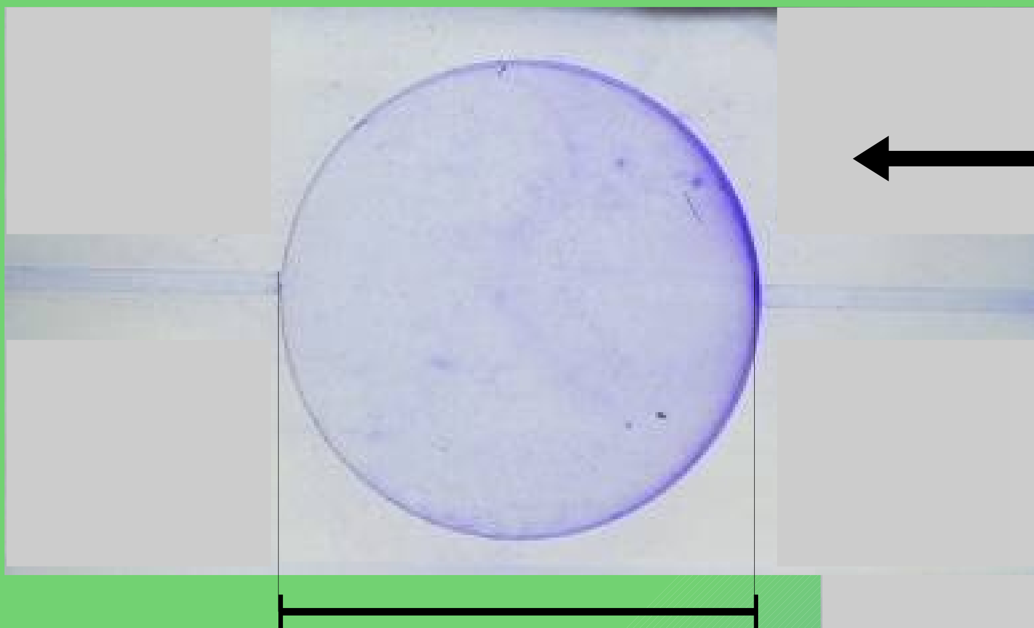
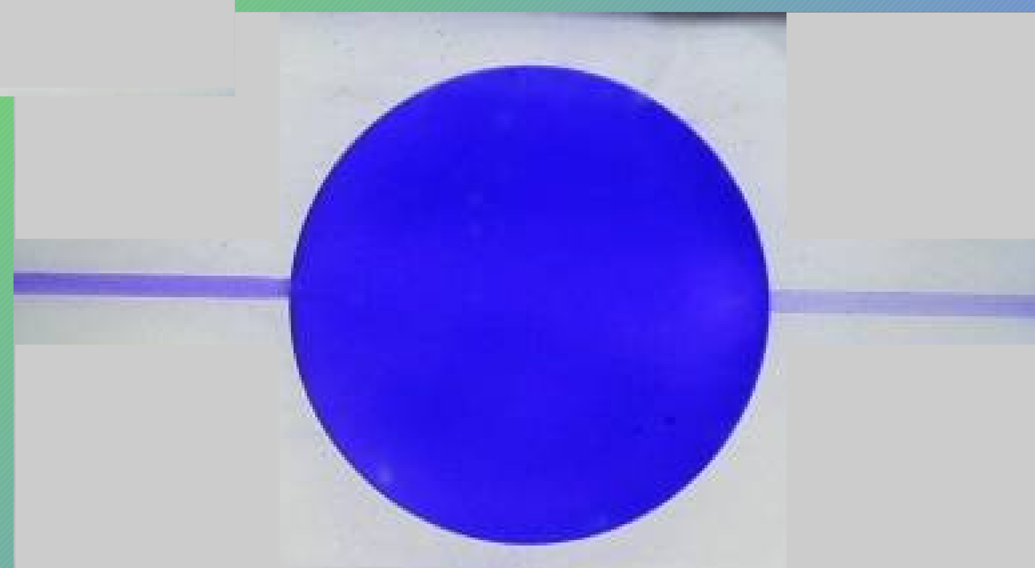


After 31.5 s of 10 ml/min water flow.



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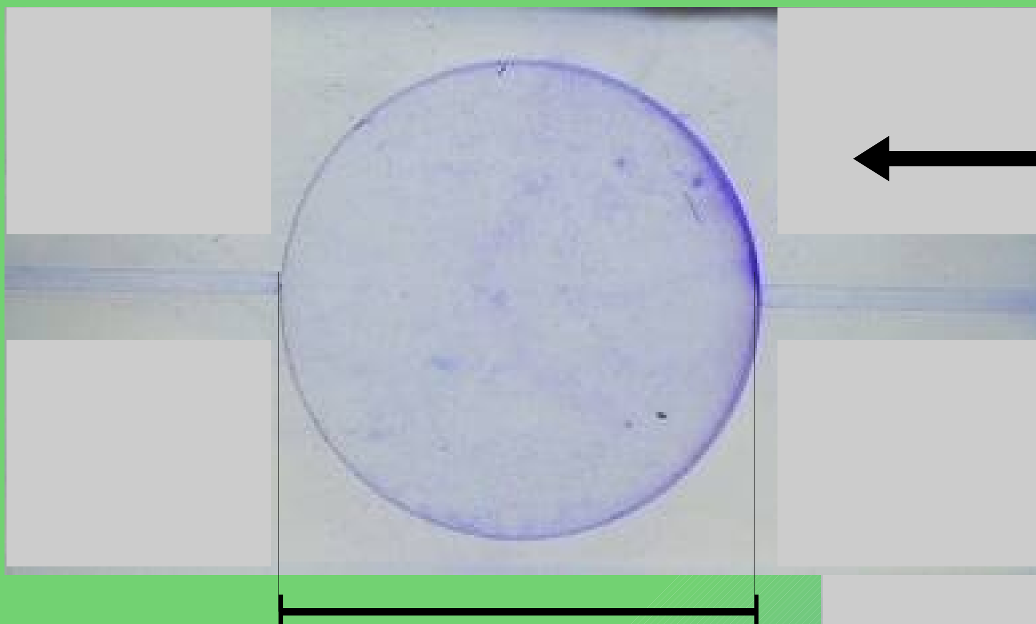
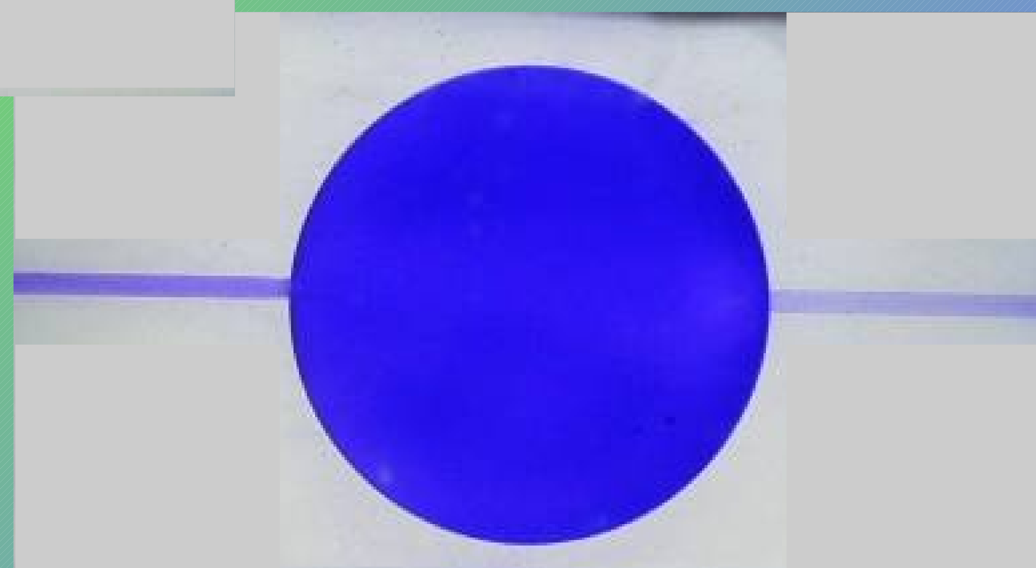


10 mm

After 36 s of 10 ml/min water flow.



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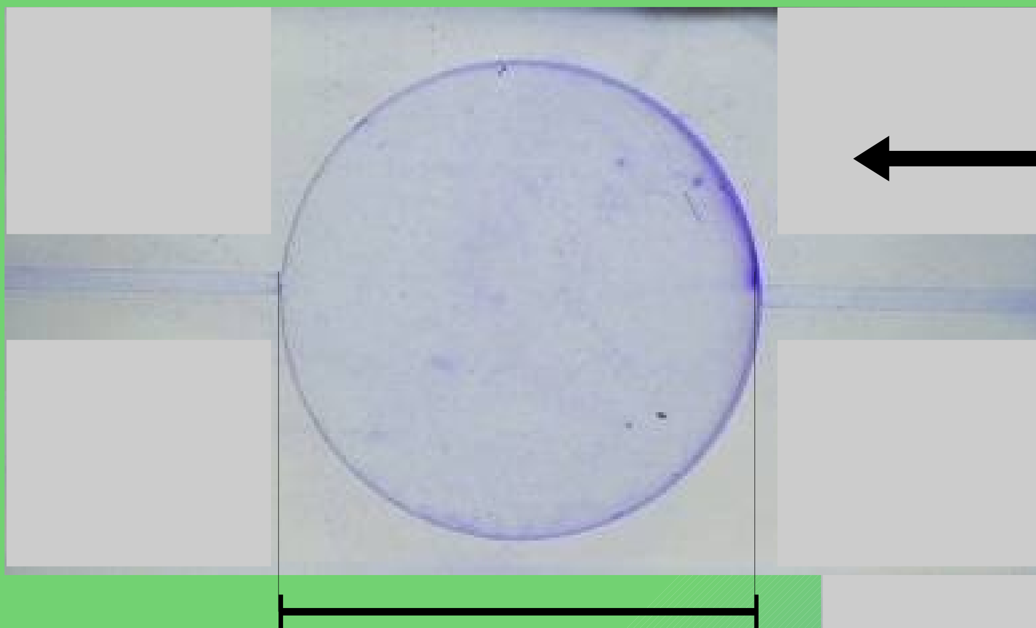
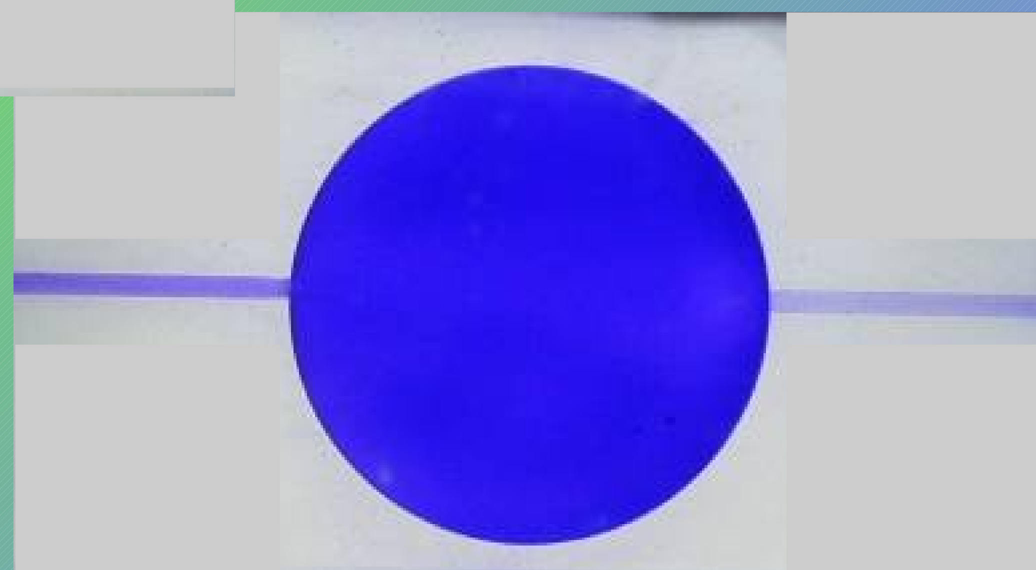


10 mm

After 40.5 s of 10 ml/min water flow.



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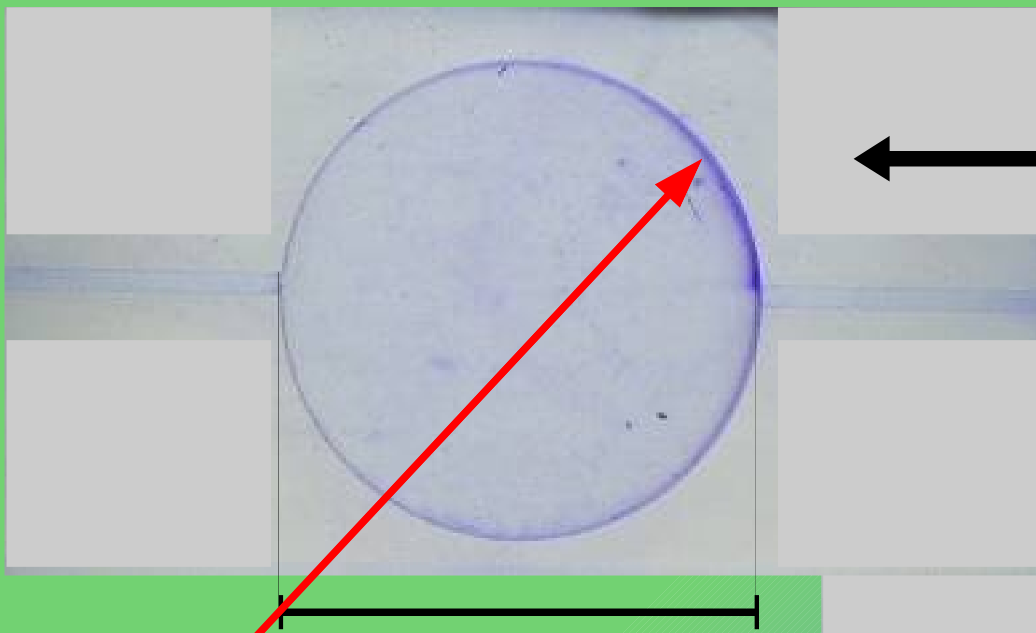
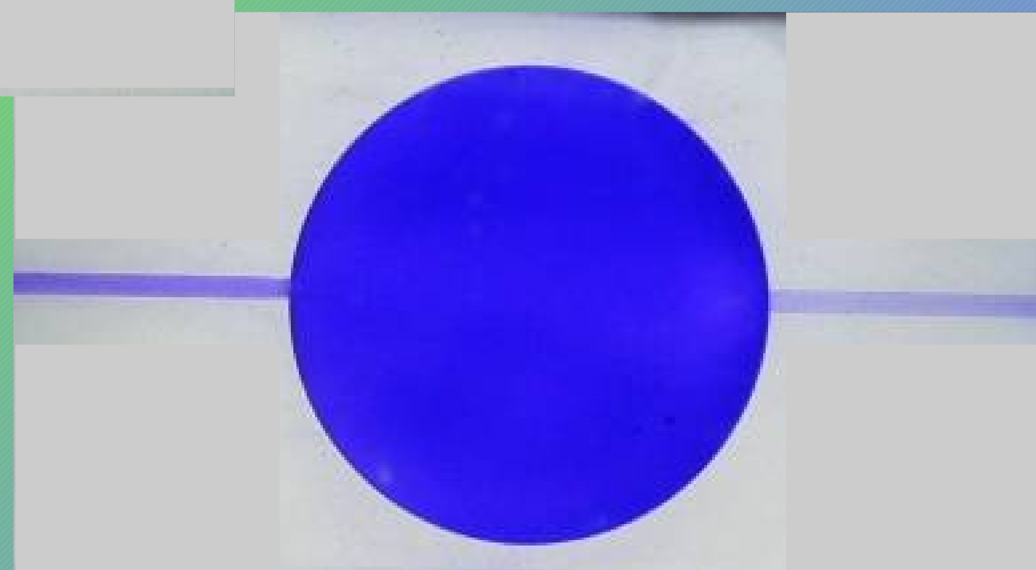


After 45 s of 10 ml/min water flow.

Almost no wash-out in region outside of convection pathways needs further flooding for several minutes until substantial washout occurs.



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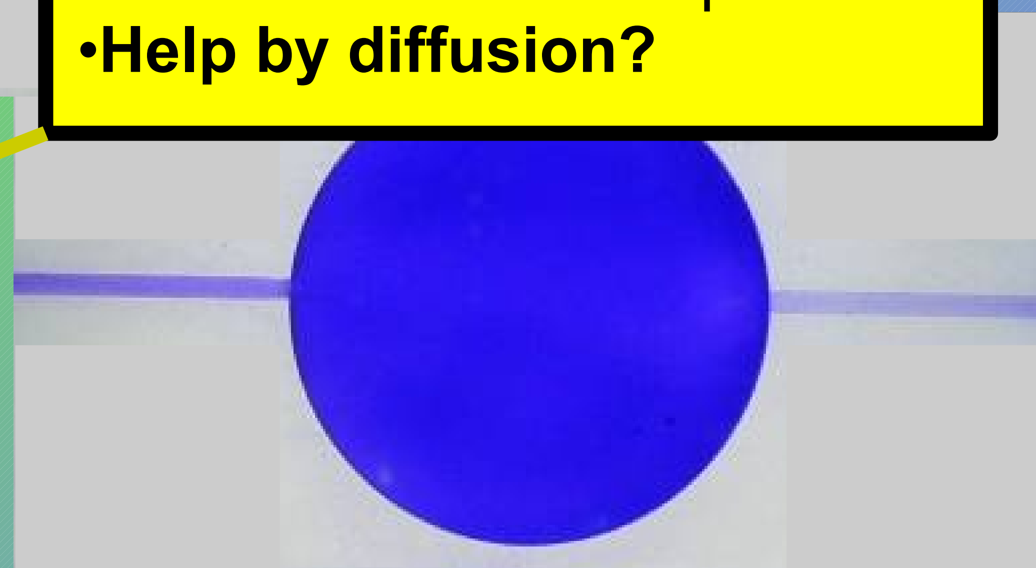
10 mm

After 45 s of 10 ml/min

- Is continous flooding really necessary?
  - Saving solvent
  - More sustainable process?
- **Help by diffusion?**



Almost no wash-out in region outside of convection pathways needs further flooding for several minutes until substantial washout occurs.

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After waiting 3 min

10 mm

Diffusive broadening of remaining
(C.I. Basic Violet 3)

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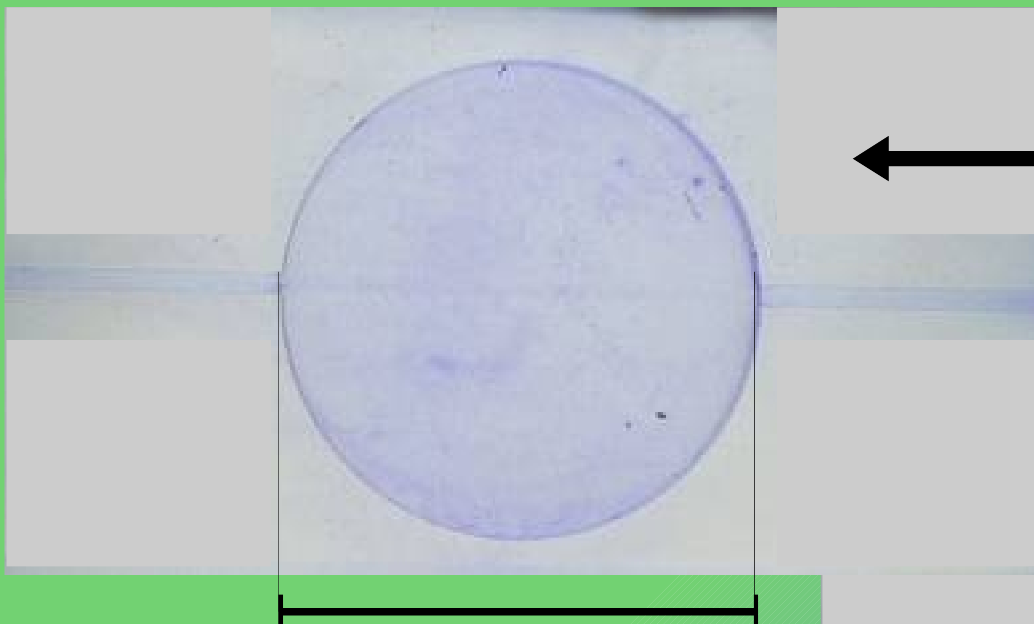
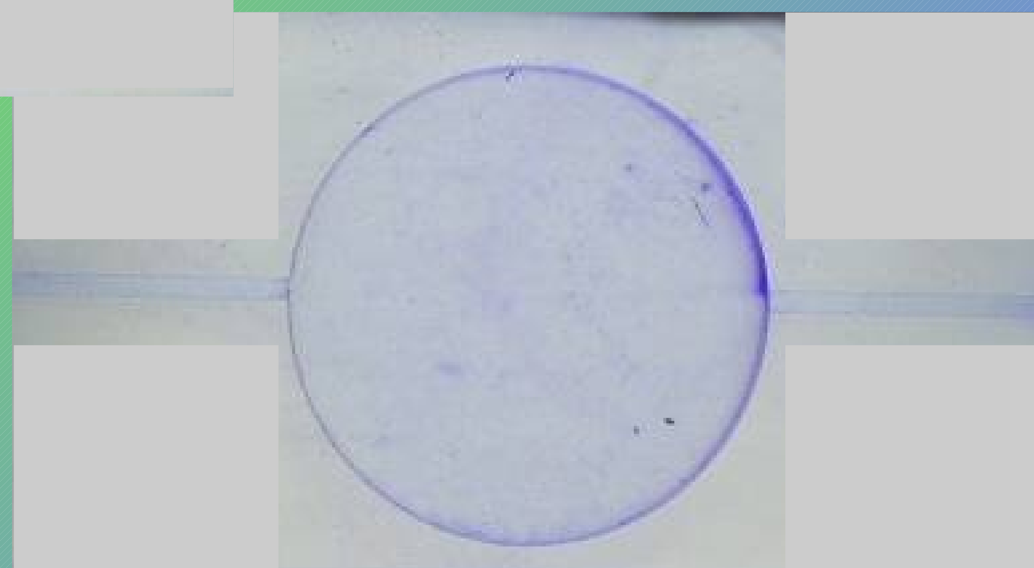


After 15 s of subsequent flooding



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Example shows: clever division of work between flow and diffusion helps saving resources

- Heterogeneous catalysis
- Adsorption and ion exchange (Posters C4, C8,...)

- Environmental remediation (Talk Barker, Poster F4)

- Chromatography (Poster C11)
- Lab on a chip

- Living organisms (Posters D6, D7)

Ringrazio tanto!

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