EPFL

Process Intensification and Green Chemistry

Mixing in microchannels

EPFL
Master of Science in Chemical Engineering and Biotechnology
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    - Engulfment
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    - Pressure drop, power dissipation, shear rate
    - Mixing time prediction
    - Comparison with experimental data
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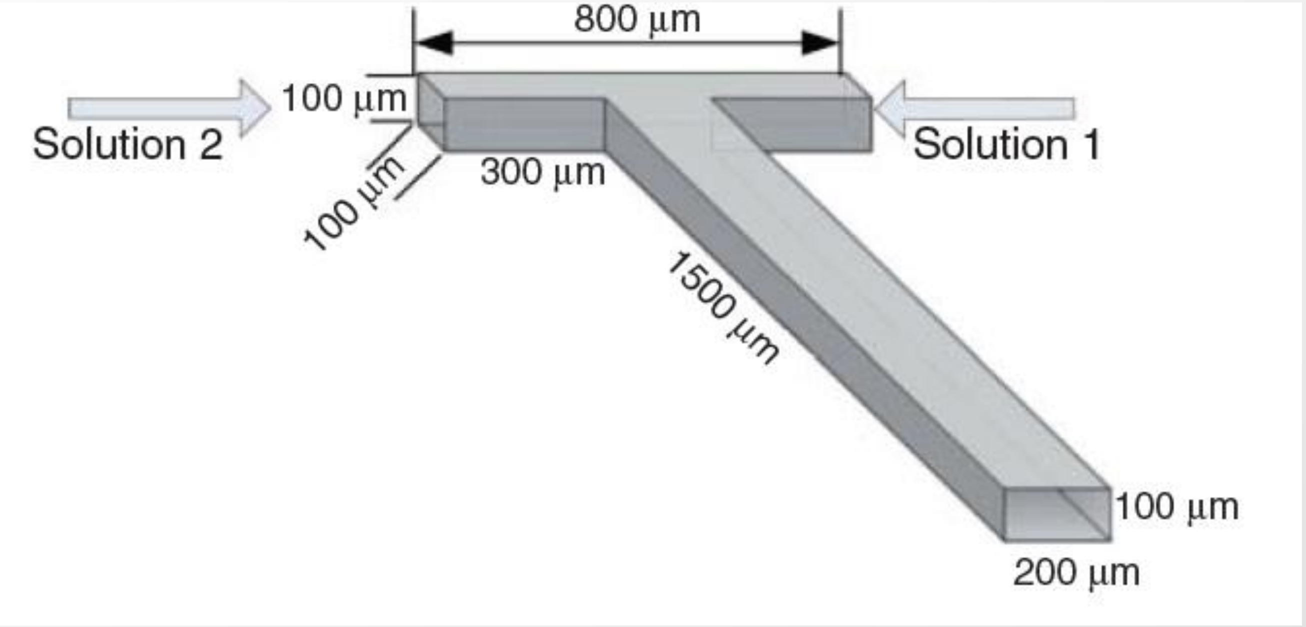
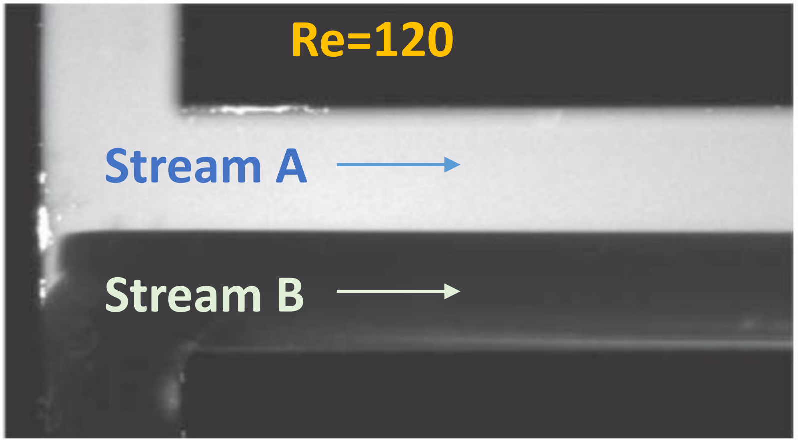
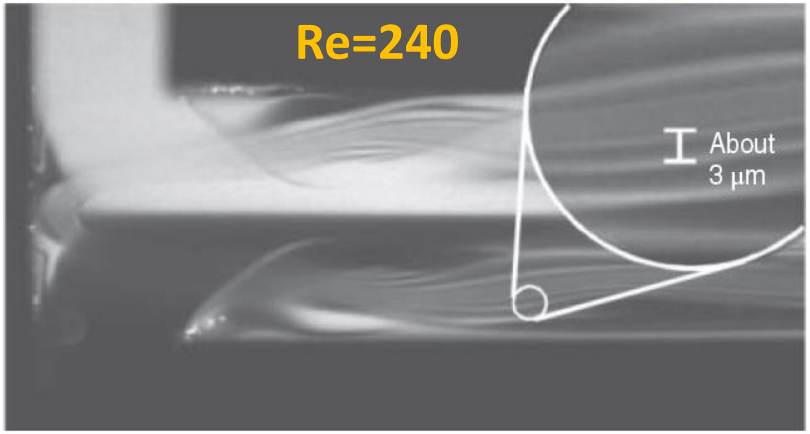
Rectangular T-mixer



Flow in T-mixer (smooth channels)





Stratified flow (Re < ~100)

- Thick liquid layers

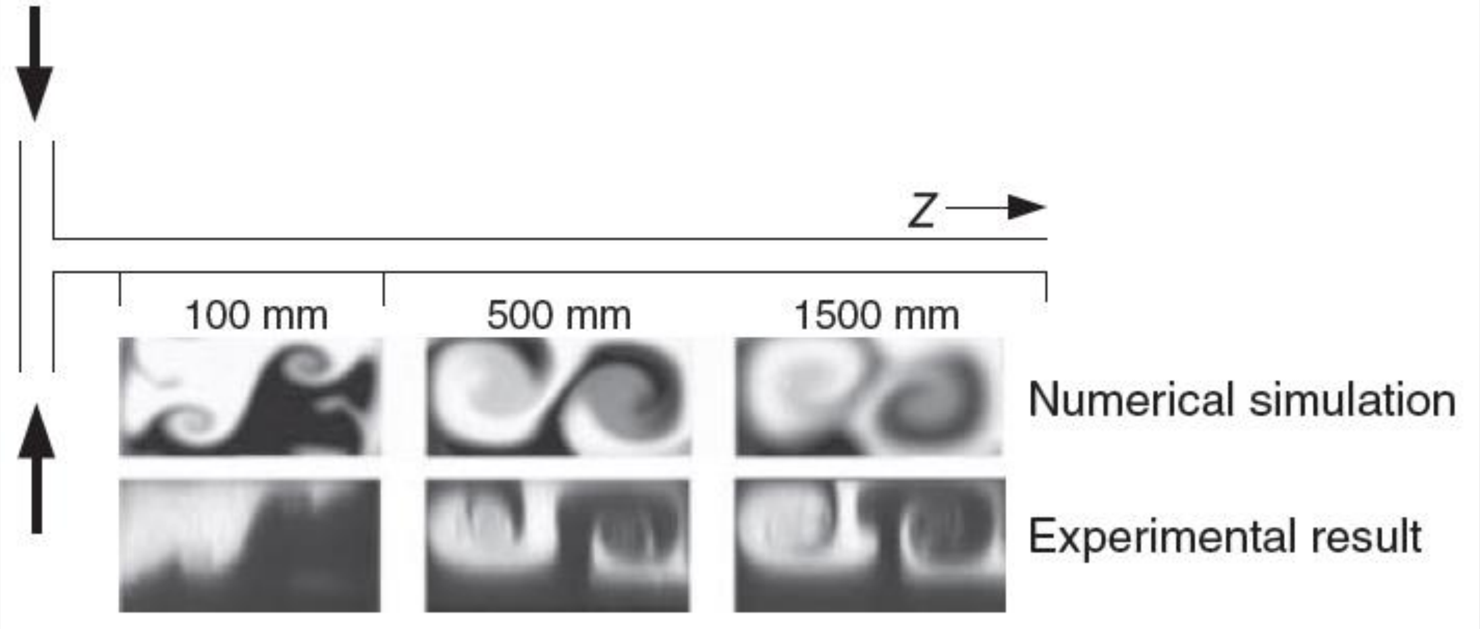
⇨ Slow mass transfer, solely controlled by diffusion

Engulfment regime (Re > ~100)

- Stretching, thinning, wrapping (intertwining) of lamellae
- Higher interfacial area
- Diffusion and convection contribute to mixing

⇨ Enhanced mass transfer

Engulfment regime for flow in T-mixer (smooth channels)



Engulfment regime
Stretching, thinning, wrapping of lamellae

Stratified flow in laminar regime: mixing by molecular diffusion

Characteristic time for diffusion: $t_{diff} = A\frac{R^2}{D}$

R: half-thickness of aggregate

A: shape factor $A = \frac{1}{(p+1)(p+3)}$

p (shape parameter): 0 for slab, 1 for cylinder, 2 for sphere

Diffusion time in water ($D=10^{-9}\ m^2\ s^{-1}$)

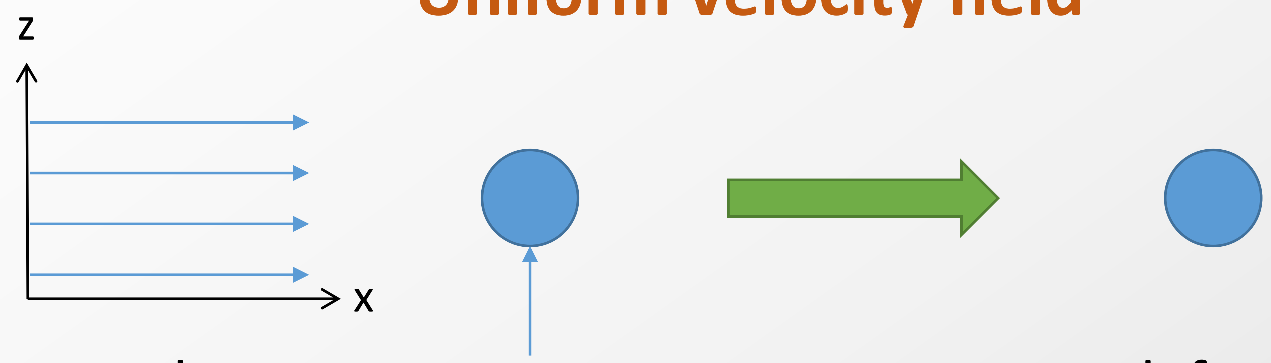
Size of slab, R	**Diffusion time**
1 mm	5 min
500 μm	1.5 min
100 μm	3 s
50 μm	**0.8 s**

Mixing in microstructures

- 50 μm is the low end of industrially feasible processes
- Blockage and/or excessive pressure drops might occur at lower sizes
- Flow regime at $R \geq 50\ \mu m$ is generally stratified ($Re < 100$) ⇨ mixing occurs only by molecular diffusion
- Mixing time in liquids at $R = 50\ \mu m$ is ~1 s, i.e. far higher than many fast reactions with characteristic times of milliseconds
- If faster mixing is required: mechanical energy necessary to reduce blob sizes below 50 μm ⇨ use of turbulent flow field would work but would imply rather high power dissipation
- In microstructures, Re mostly $<\ 1000$ (laminar) but mixing in laminar a flow field can still be very efficient thanks to the occurrence of the engulfment regime

Laminar mixing in a shear field

Uniform velocity field



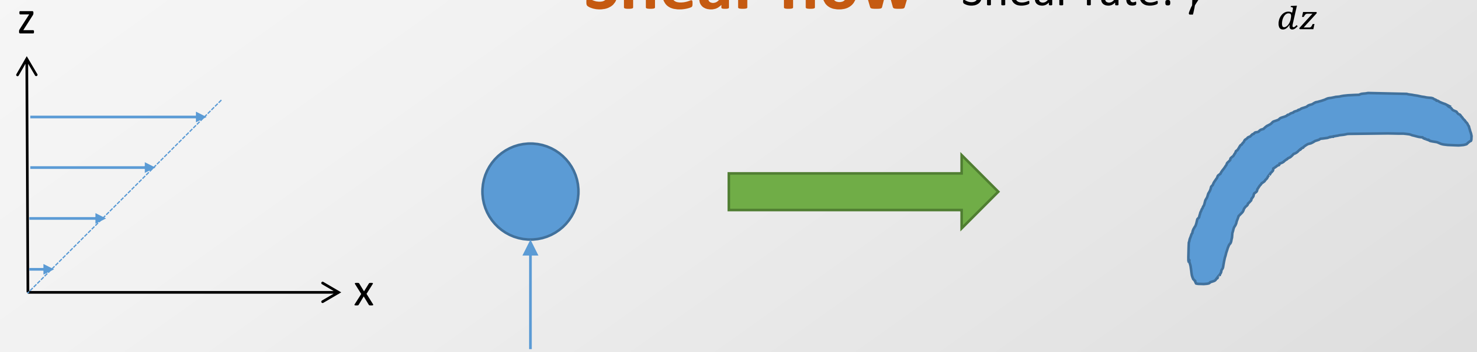
No shear

Fluid particle

No deformation

Shear flow

Shear rate: $\dot{\gamma} = \frac{du}{dz}$



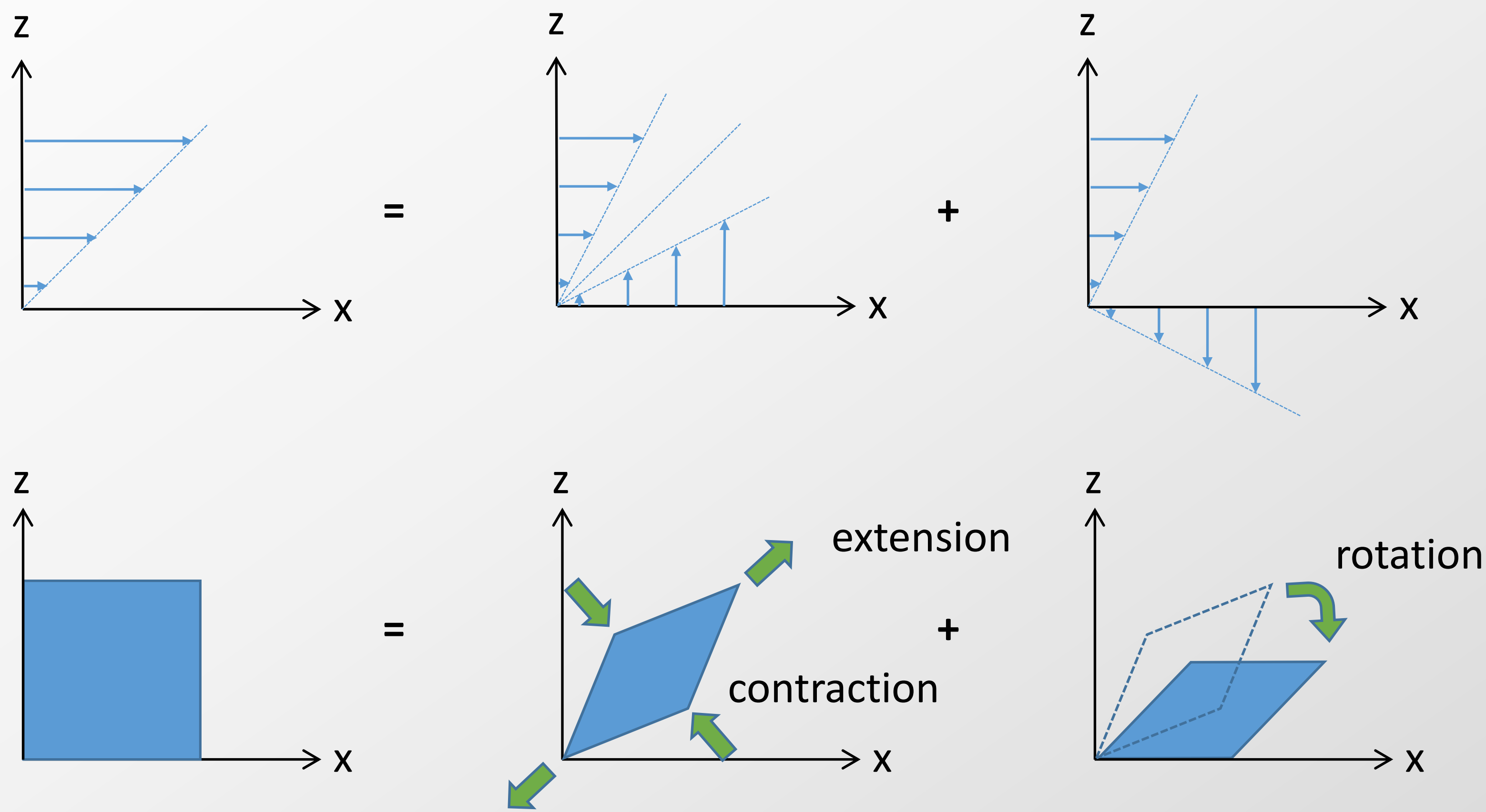
Shear flow

Fluid particle

Stretching and folding

Laminar mixing in a shear field

Shear flow = Deformation + Rotation



Laminar mixing in a shear field

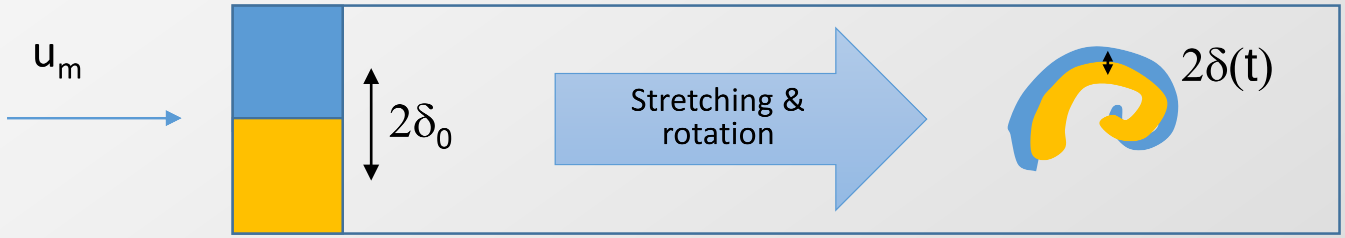
- Objective of mixing:

  Produce maximum interfacial area in the minimum amount of time using the minimum amount of energy

- Shear rate: $\dot{\gamma} = \frac{du}{dz}$

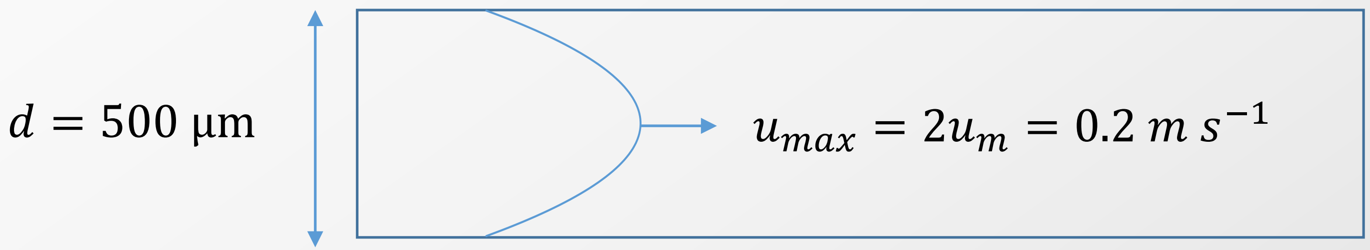
- Thickness *vs* time in a shear flow: $\frac{\delta(t)}{\delta_0} = \frac{1}{\sqrt{1+(\dot{\gamma}t)^2}}$

- As thickness decreases, concentration gradient increase, thus mass flux $(-\mathrm{D}\frac{dc}{dz})$ increases



Laminar mixing in a shear field

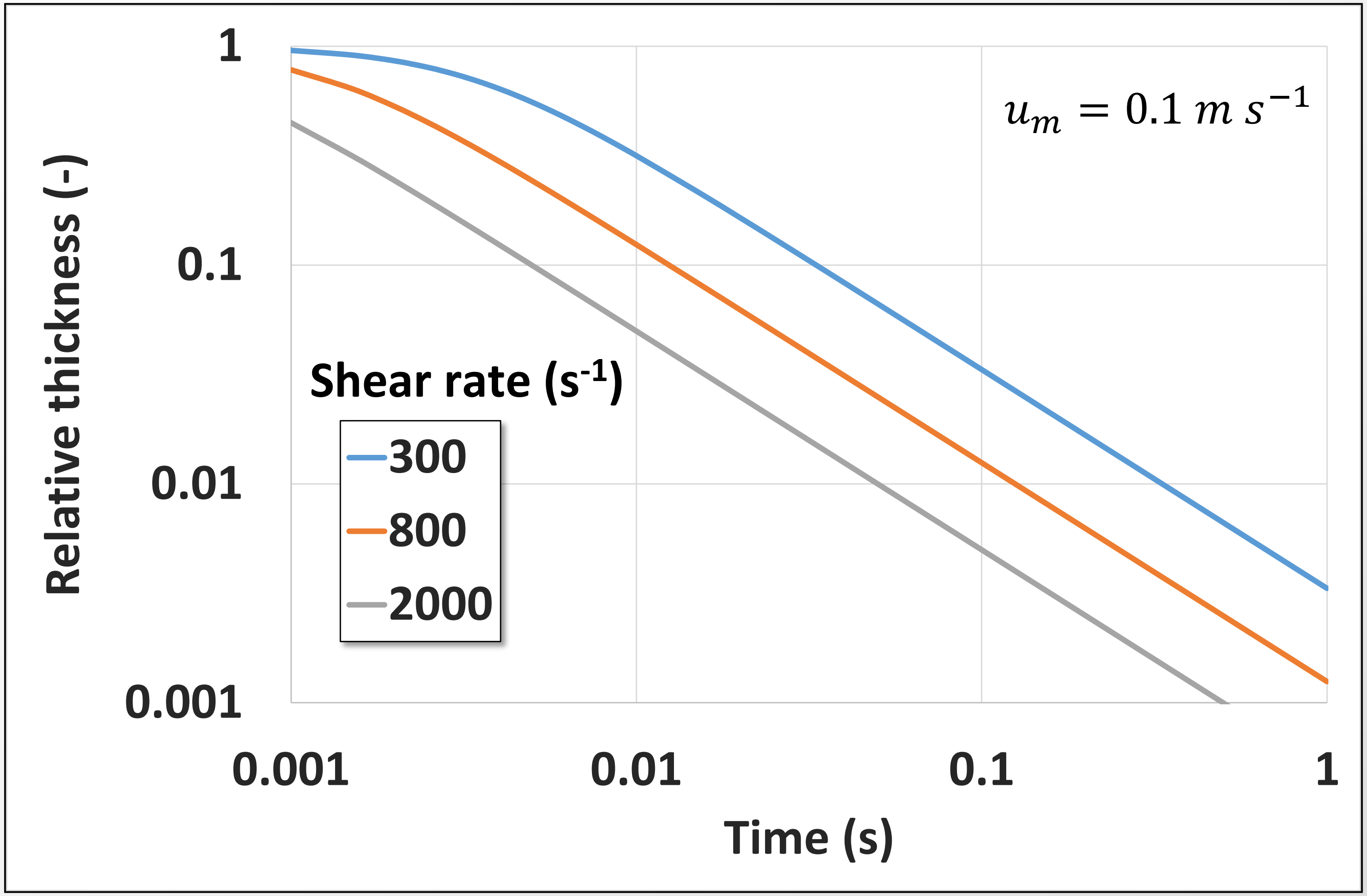
- Example: aggregate thickness in laminar flow with mean velocity (u_m) of 0.1 m/s in 500 μm microchannel



$$\dot{\gamma} = \frac{du}{dz} = \frac{2u_m}{R} = \frac{2 \cdot 0.1}{\frac{500\ 10^{-6}}{2}} = 800\ s^{-1}$$

⇨ Thickness is 10% of initial value in 10 ms (next slide)

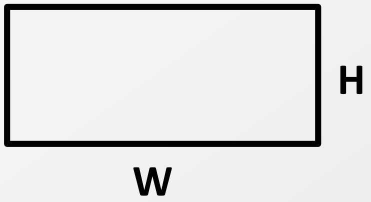
Laminar mixing in a shear field



Key variables in circular microchannel (laminar flow)

- Pressure drop: $\frac{\Delta p}{L} = \frac{32\mu u_m}{d^2}$
- Specific power dissipation: $\varepsilon = \frac{Q\Delta p}{\rho V} = \frac{8\nu u_m^2}{R^2}$
- Mean shear rate: $\dot{\gamma} = \frac{2u_m}{R} = \sqrt{\frac{\varepsilon}{2\nu}}$

Pressure drop in rectangular microchannel (laminar flow)



- Pressure drop: $\frac{\Delta p}{L} = \xi \frac{32 \mu u_m}{d_h^2}$
- Hydraulic diameter: $d_h = 4 \frac{\text{cross-sectional area}}{\text{perimeter}} = 2 \frac{HW}{(H+W)}$
- Geometric factor for rectangular channels:

$$\xi = 0.8735 + 0.6265\, exp\left(-3.636 \frac{H}{W}\right)$$

- Square channels: $\xi = 0.85$
- Circular channels: $\xi = 1$ and $d_h = d_t$
- Specific power dissipation: $\varepsilon = \frac{Q \Delta p}{\rho V} = \xi \frac{32 \nu u_m^2}{d_h^2}$

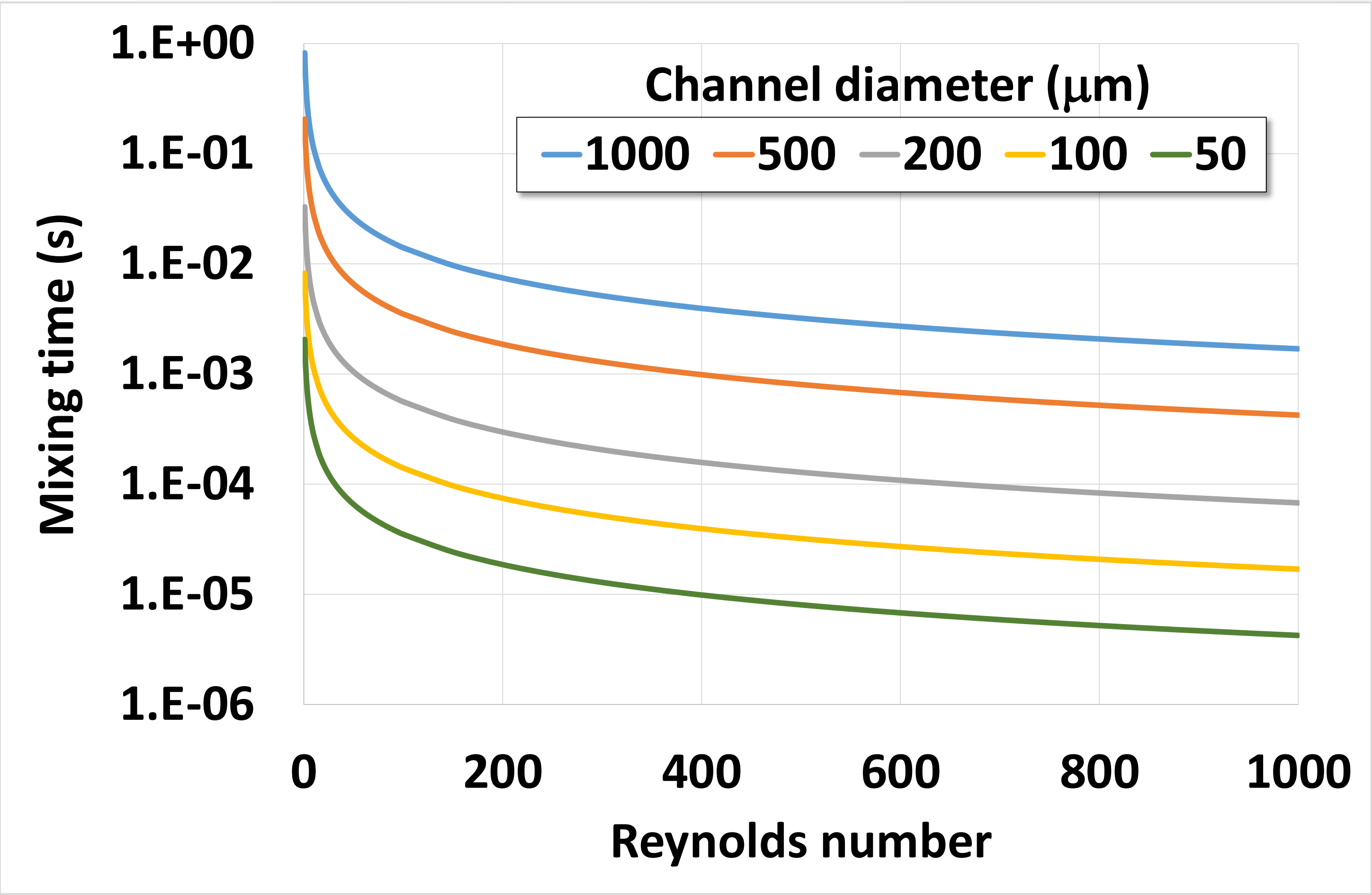
Predicted mixing time in microchannel (laminar flow)

- General equation (diffusion in shear flow, intertwined lamellae):
  - $t_{mix} = t_{diff+shear} = \frac{1}{2\dot{\gamma}} arcsinh\left(\frac{0.76\dot{\gamma}\delta_0^2}{D}\right)$

- Tubular geometry:
  - $t_{diff+shear} = \frac{d}{8u_m} arcsinh(0.76 \cdot Pe)$ $\left(Pe = \frac{u_m d}{D}\ ;\ \delta_0 = \frac{d}{2}\right)$
- Tubular geometry, liquids (Sc>>1)*:
  - $t_{diff+shear} = \frac{d^2}{8DPe} ln(1.52 \cdot Pe) = \frac{1}{\sqrt{2}}\sqrt{\frac{\nu}{\varepsilon}} ln(1.52 \cdot Pe)$
  - $t_{diff+shear} \cong 0.0075 \cdot \varepsilon^{-0.5}$ (water, see next slides)

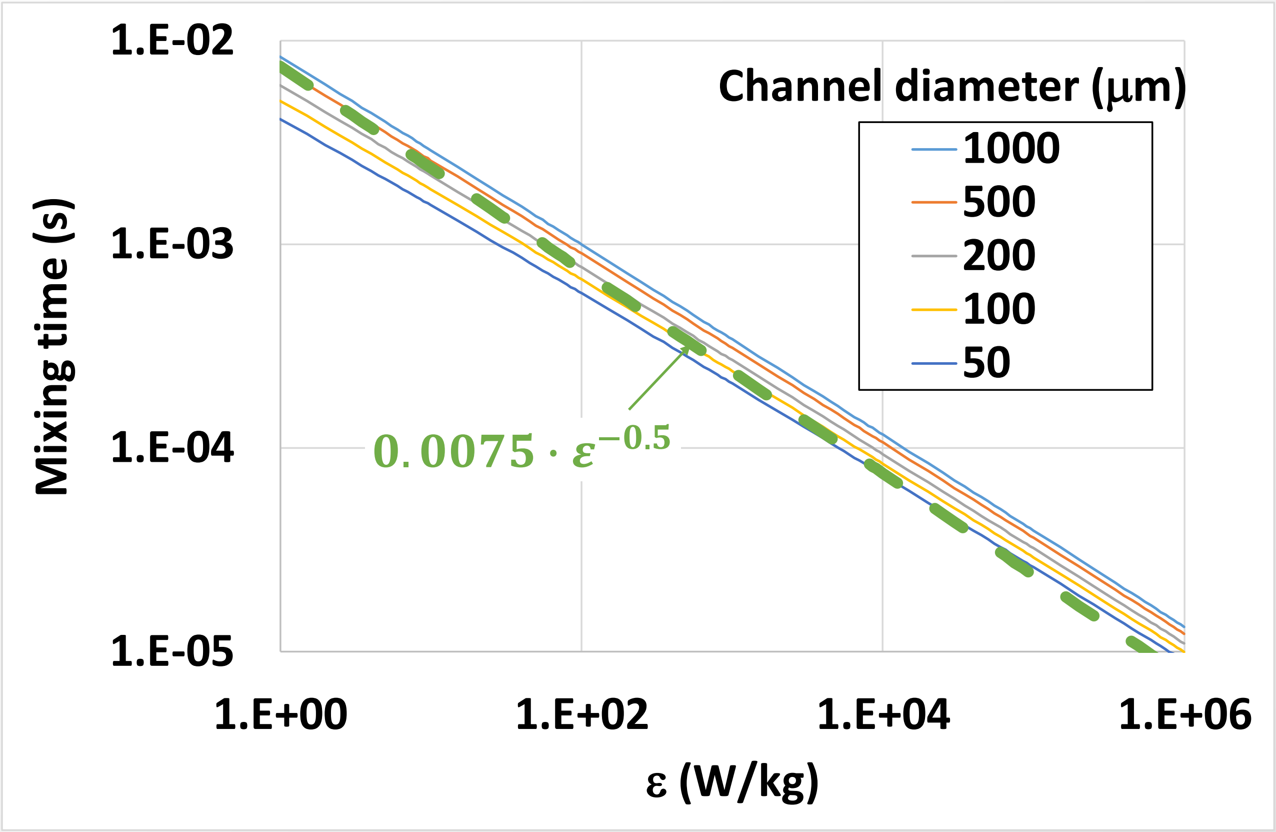
$*for\ x >\sim 5\text{: } \text{arcsinh}(x) = \ln(2x)$

Predicted mixing time in microchannel (water, laminar flow)



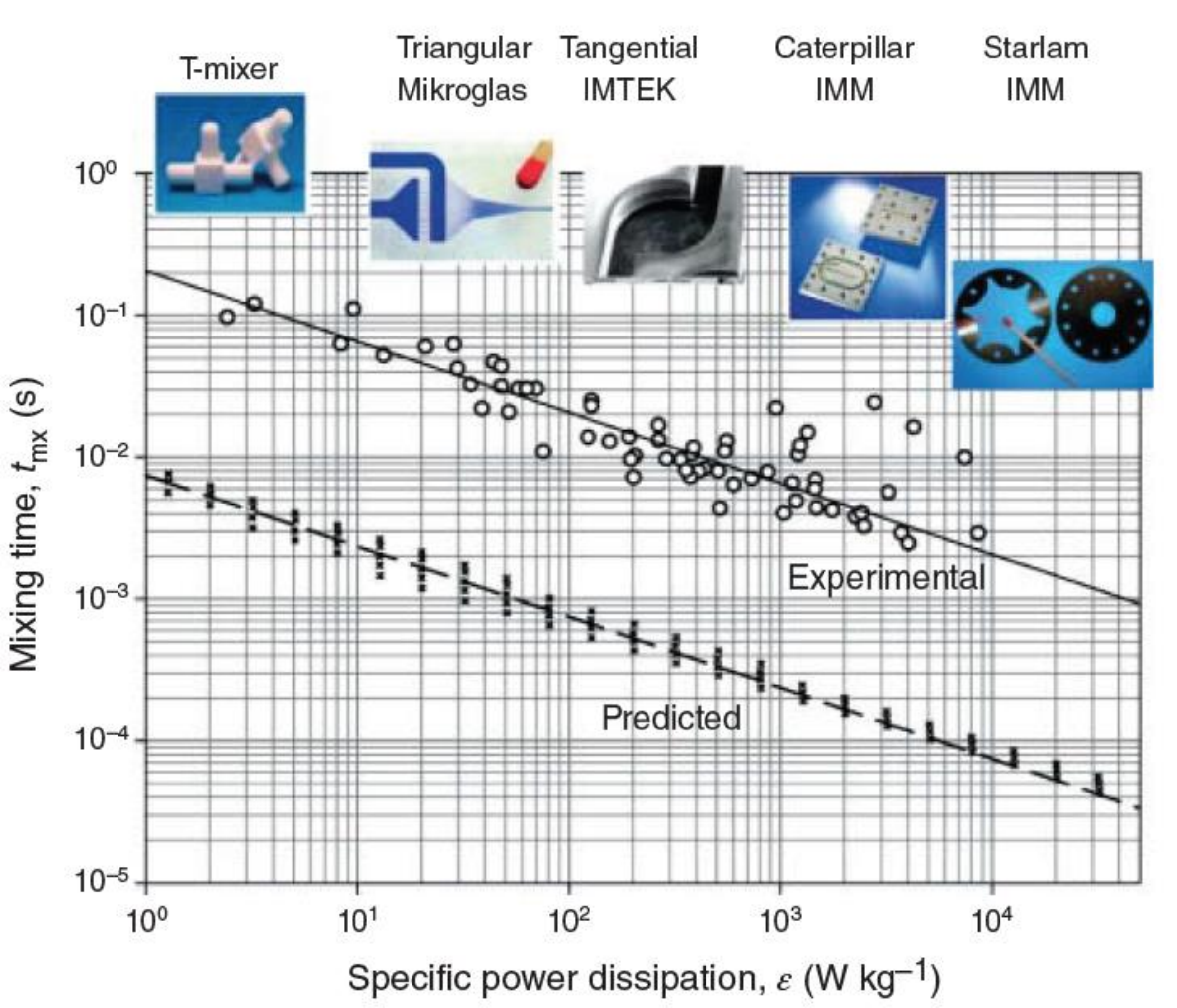
Very low mixing time achievable in theory (ms or lower)

Predicted effect of specific power dissipation (water)



- Minor effect of channel diameter
- $t_{mix}(theoretical) \cong 0.0075 \cdot \varepsilon^{-0.5}$

Experimental vs predicted mixing time in micromixers



$$t_{mx,exp} \cong 0.215 \cdot \varepsilon^{-0.5}$$

$$t_{mx,pred} \cong 0.0075 \cdot \varepsilon^{-0.5}$$

Experimental vs predicted mixing time in micromixers

- Experimental mixing times are much higher than theory (~30 times)
- Mixing time depends mainly on ε, not geometry

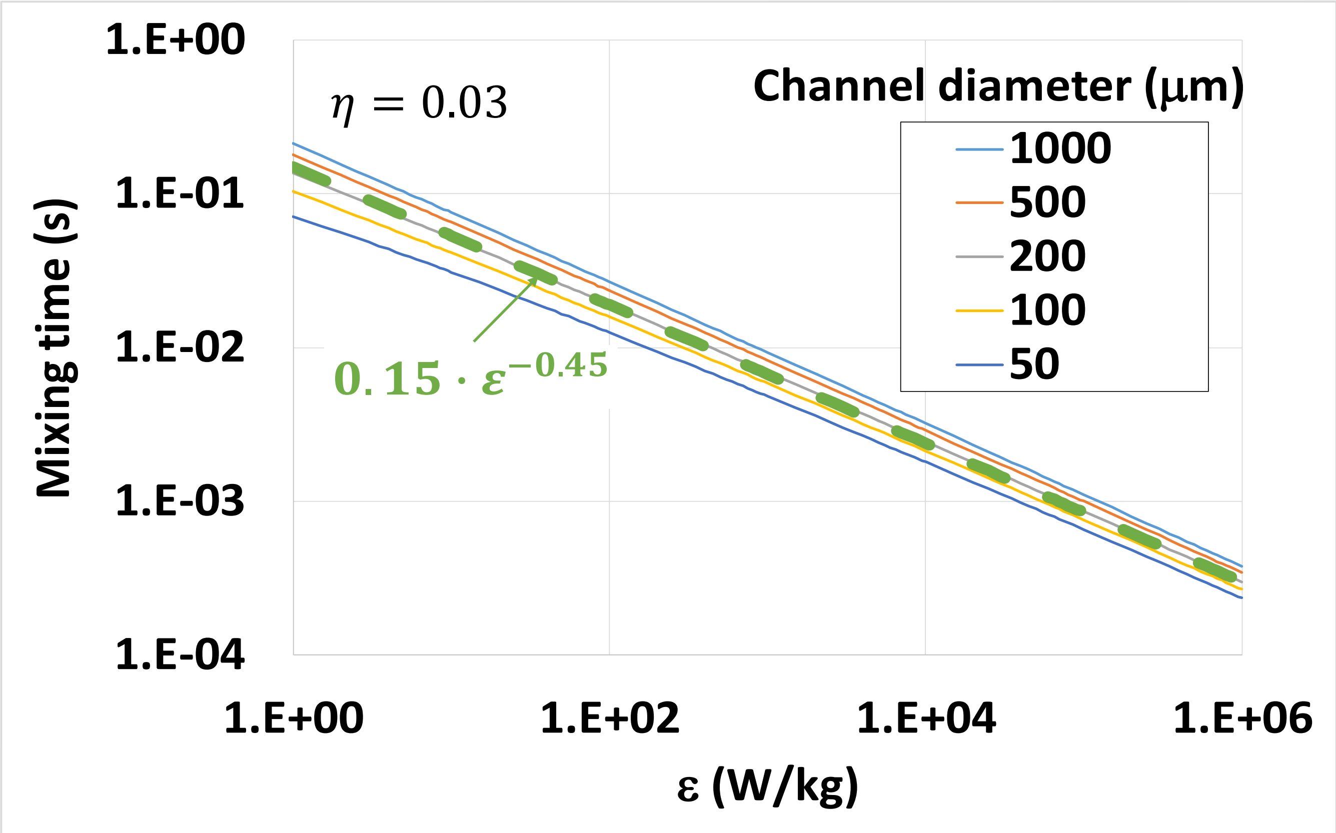
Some reasons for low mixing efficiency

- Some time required to mix the 2 flows to obtain interlaced slabs of A and B (sandwich structure)
- Non-constant shear rate as lamellae are rotated and do not experience constant deformation rate
- Sometimes lamellae are perpendicular to the stretching field → striation thickness increases → reduction in concentration gradient
- Flow field and concentration field don't match → mechanical energy wasted to mix regions of pure A or B with no A/B interface

Effect of mixing efficiency on mixing time

- Energetic efficiency of mixing η:
- $\eta = \dfrac{fraction\ of\ shear\ rate\ effectively\ used\ for\ mixing}{total\ shear\ rate\ used\ for\ the\ flow}$
- $\eta = \dfrac{\dot{\gamma}}{\dot{\gamma}_{max}} = \dfrac{\dot{\gamma}}{\sqrt{\varepsilon/(2\nu)}}$
- $t_{diff+shear} = \dfrac{d}{8u_m\eta}\ ln(1.52Pe\ \eta)$
- $t_{diff+shear} = \sqrt{\dfrac{32\nu}{\eta^2\varepsilon}}\ ln\left(1.52\sqrt{\dfrac{\varepsilon}{32\nu^3}}d^2\eta Sc\right)$

Mixing time prediction with 3% efficiency



Data for channel diameters between 50 and 1000 µm with $\eta = 0.03$: well described by power law $t_{diff+shear} = 0.15 \cdot \varepsilon^{-0.45}$