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Simulation of chromatographic band transport

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Outline

1. About chromatography
2. Detector cell: Band transport in open fluid

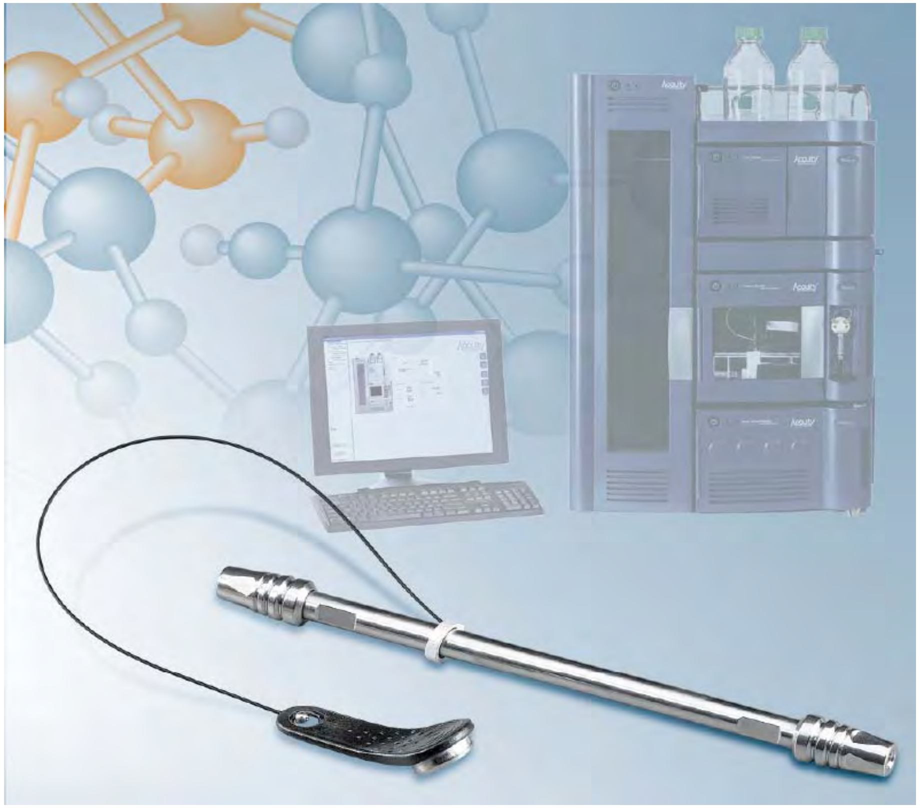
   → Navier-Stokes + convection-diffusion
3. Microfluidic chip: Band transport in a packed bed:

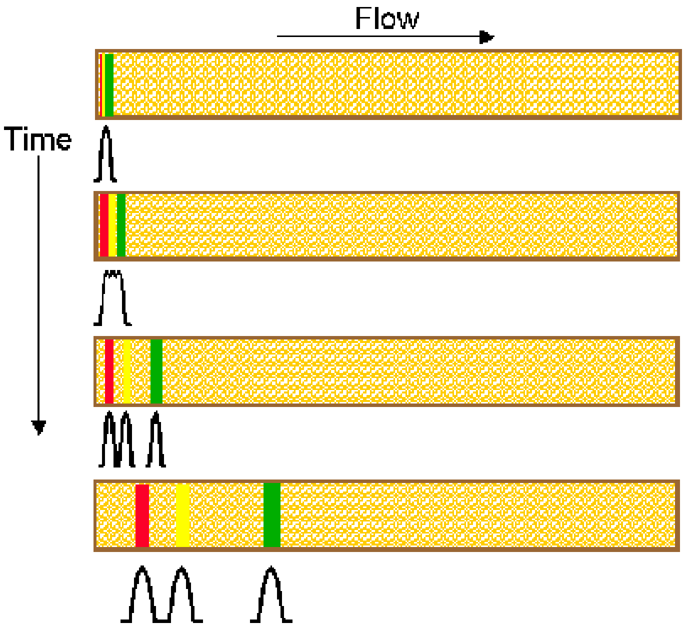
   + Darcy's law
4. Thermal effects in 2.1 mm column

   + heat equation

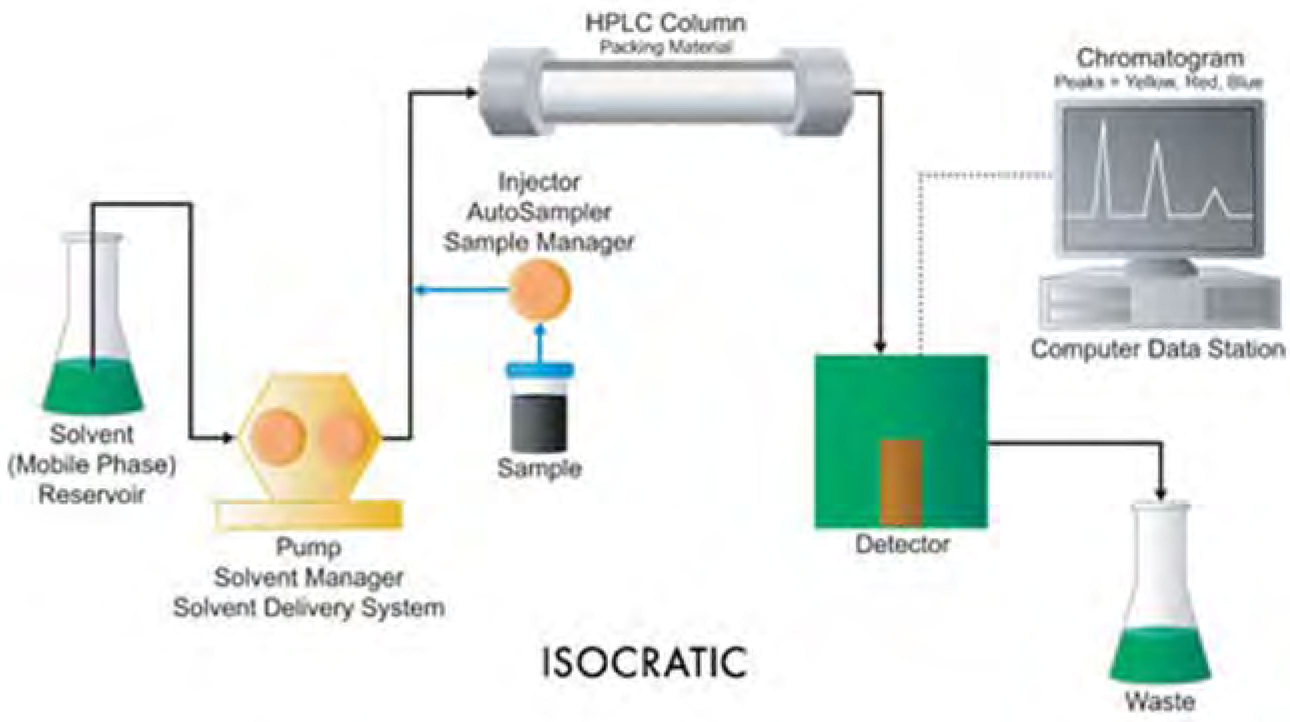
What is chromatography?

- Pass a mixture of chemical species dissolved in a liquid mobile phase through a stationary phase physically located in a column
- Depending on chemical affinity of the different species with the stationary phase, they elute at different times ⇒ <u>separation</u>

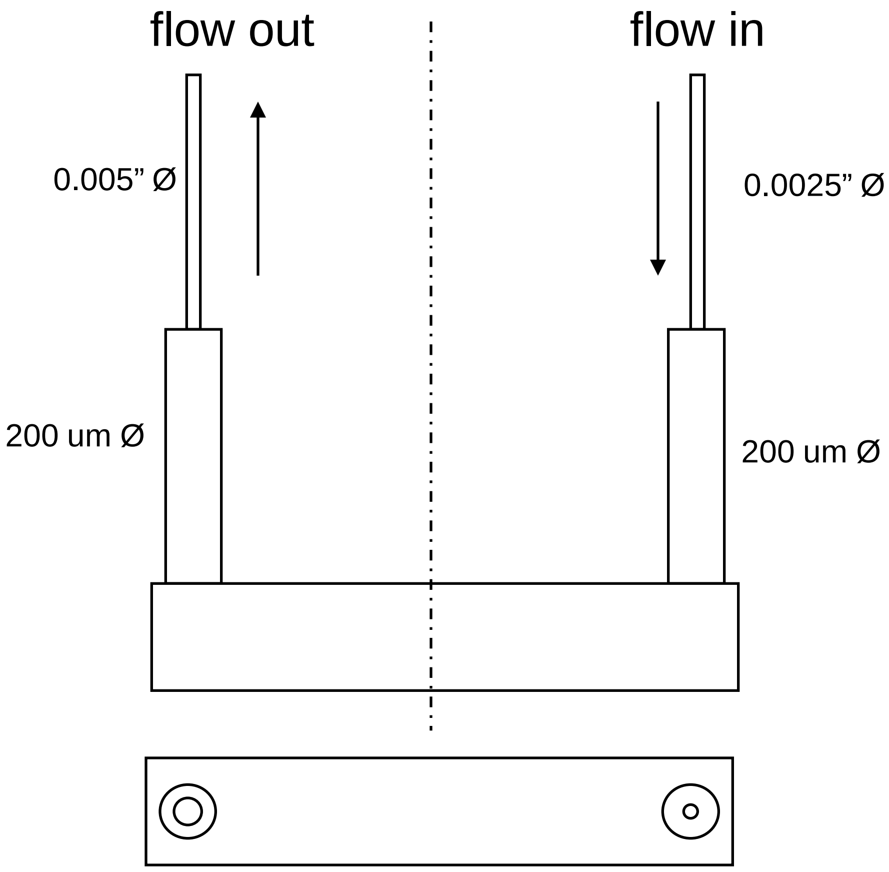




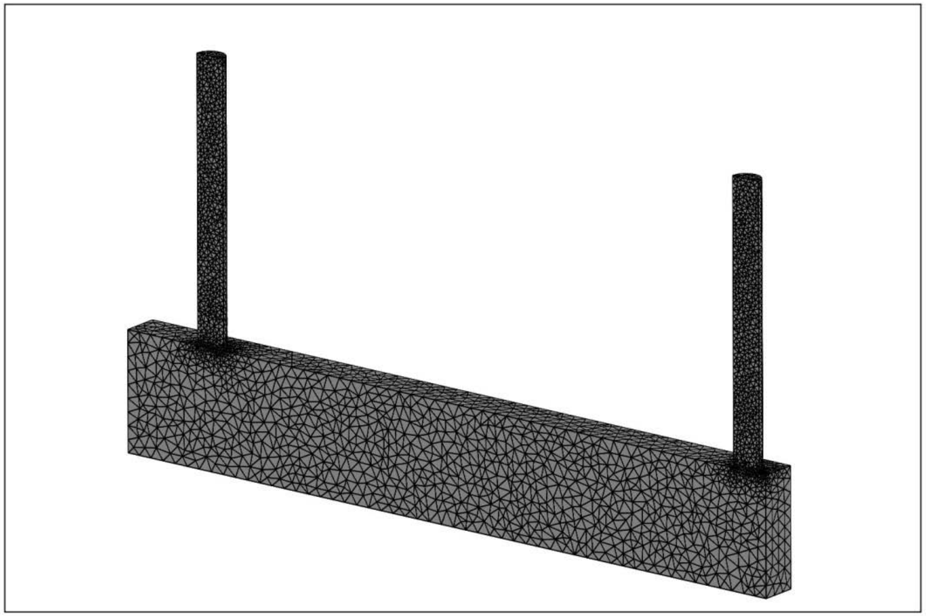
An HPLC system



Detector



geometry



mesh

Governing equations

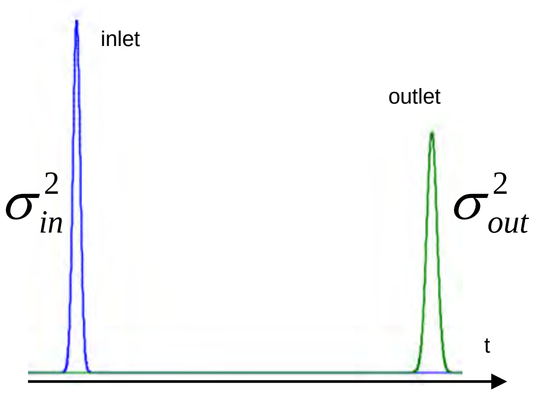
- Incompressible Navier-Stokes

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho\,\vec{u}.\nabla\vec{u}=\mu\nabla^2\vec{u}$$

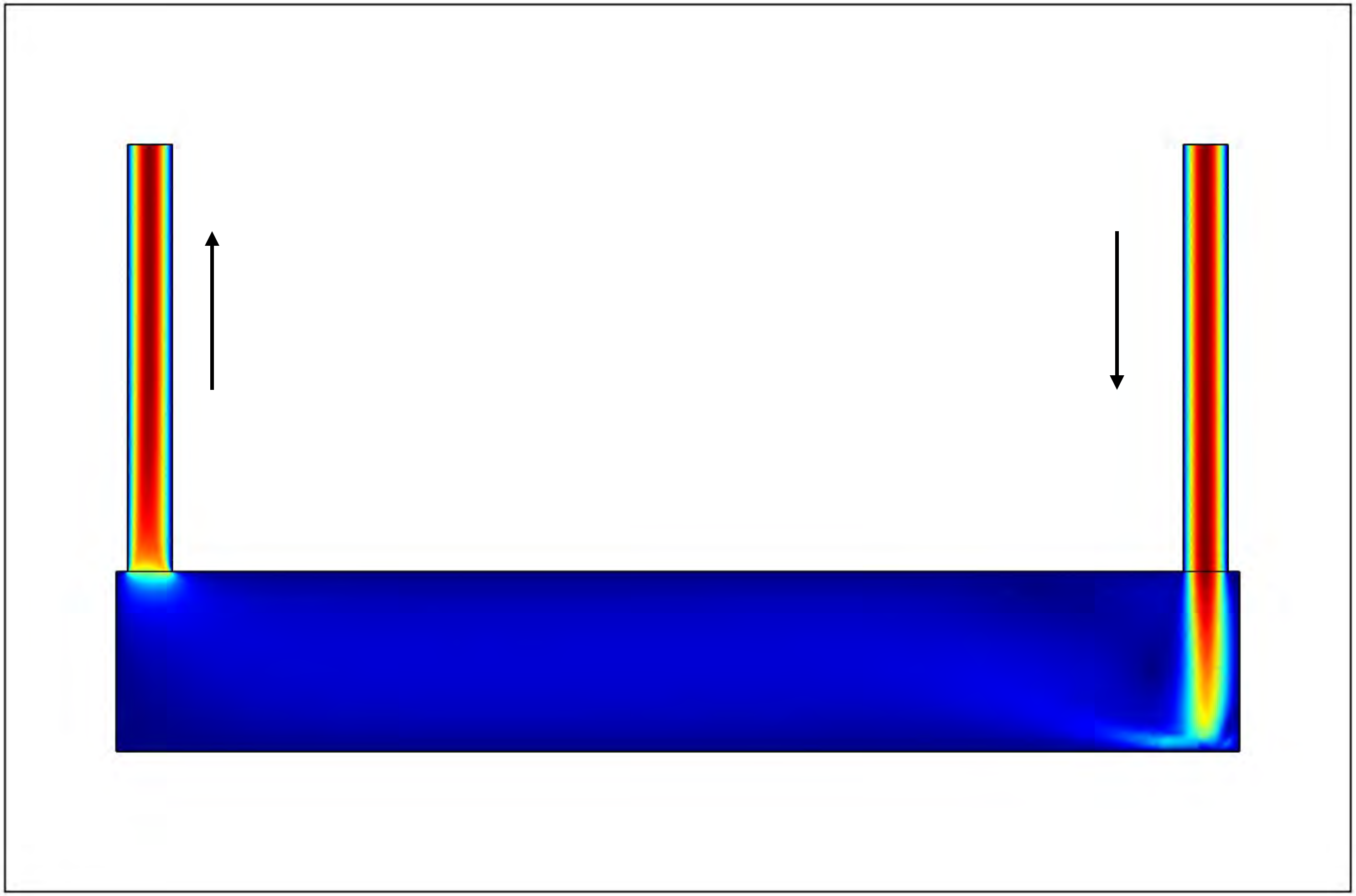
- Convection-diffusion for analyte band

  numerical vs physical diffusion

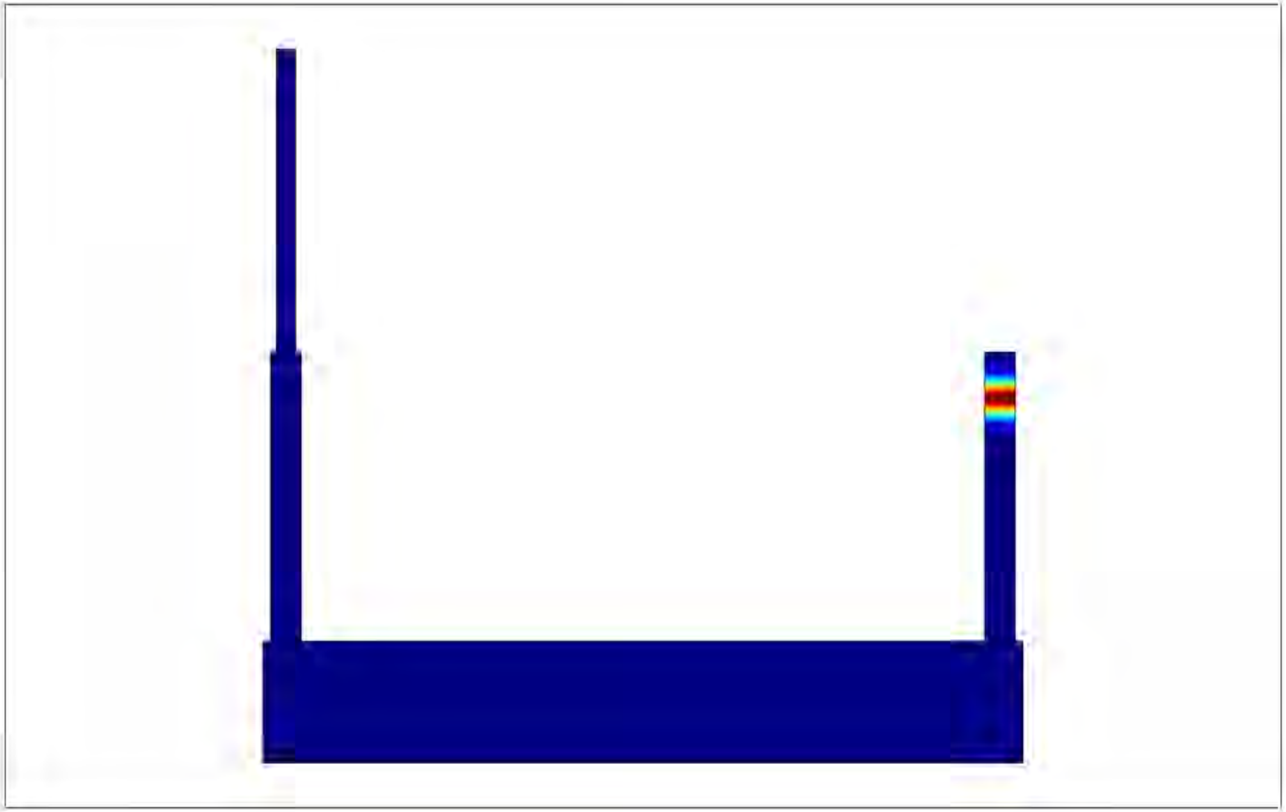
$$\frac{\partial C}{\partial t}+\vec{u}.\nabla C=D\nabla^2 C$$



Velocity field



Band transport

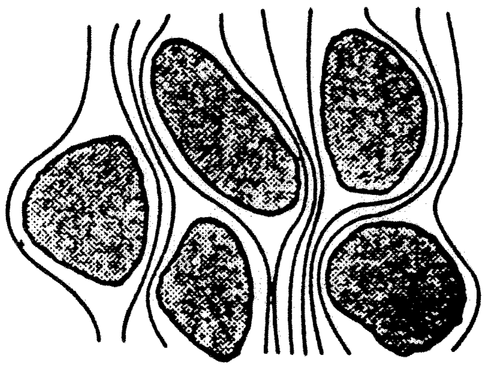


Transport in a packed bed

- Solvent: Darcy's law $\nabla^2 P = 0$

  superficial velocity $\vec{U}_s = -\frac{k}{\mu}\nabla P$

  permeability $k = \frac{d_p^2 \varepsilon^3}{180(1-\varepsilon)^2}$ void fraction $\varepsilon = \frac{V_m}{V_{tot}}$



- Solute:

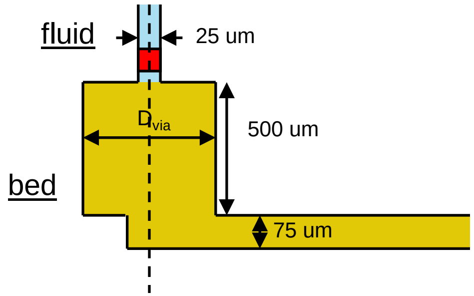
  linear velocity $\vec{u} = \frac{\vec{U}_s}{\varepsilon_t}$

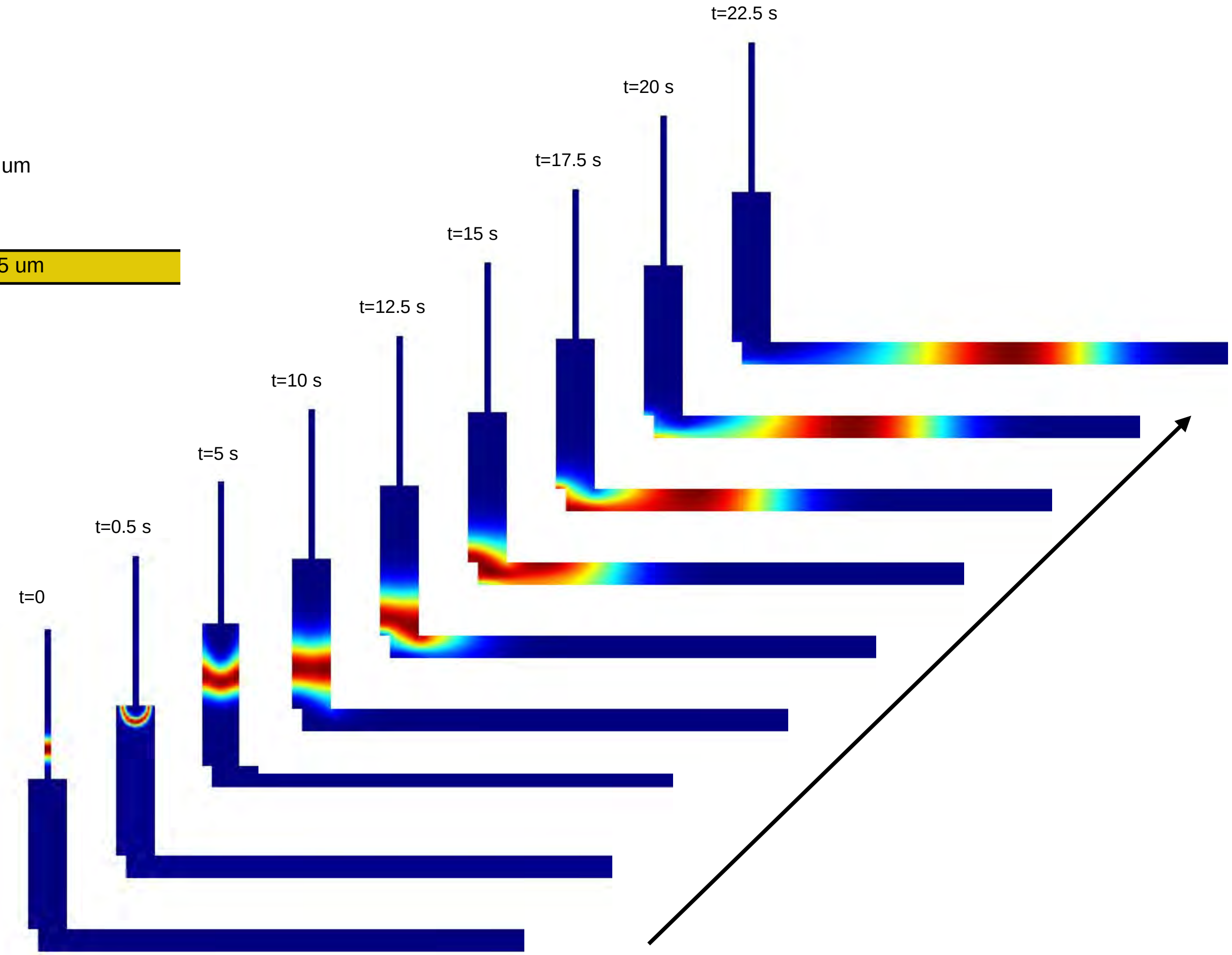
  evolution of concentration $\frac{\partial C}{\partial t} + \vec{u}.\nabla C = D_{eff}\,\nabla^2 C$

  effective diffusion coefficient $D_{eff} = \frac{H\,u}{2}$

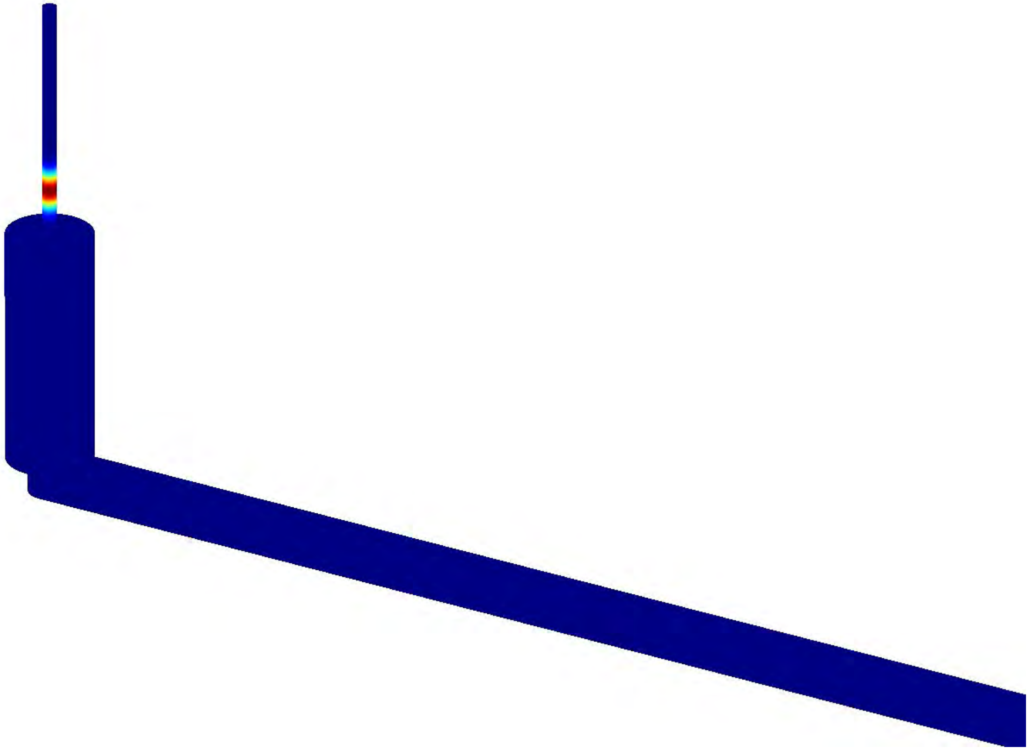
  plate height (Van Deemter) $H(u) = 1.5 d_p + \frac{D_{mol}}{u} + \frac{d_p^2}{6D_{mol}}u$

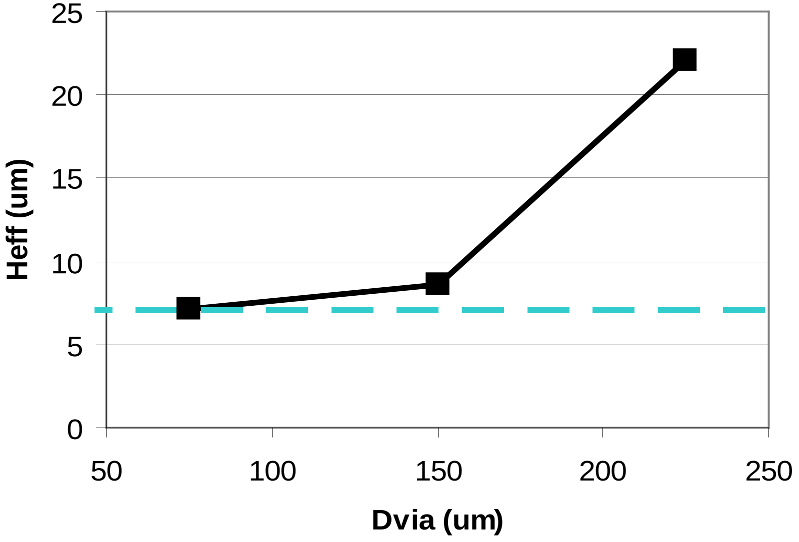
Microfluidic chip: inlet/outlet vias



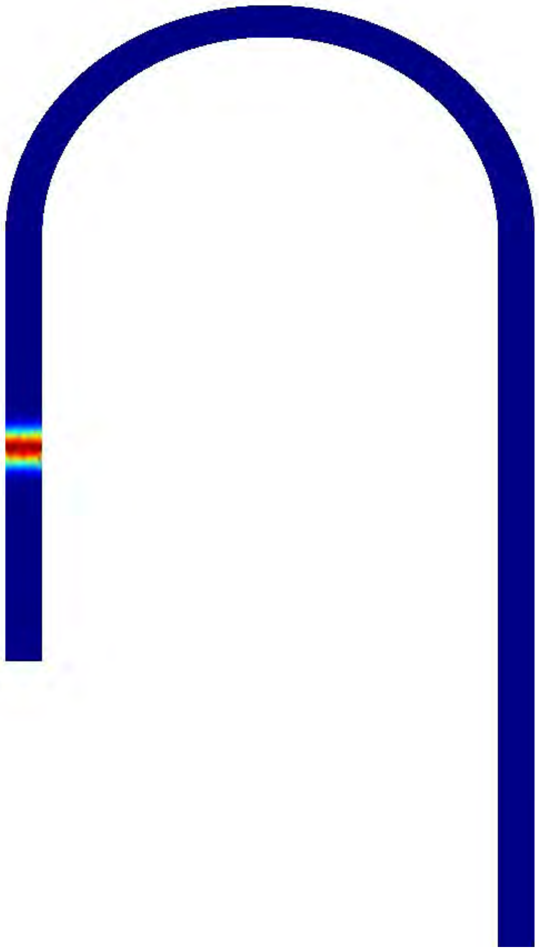


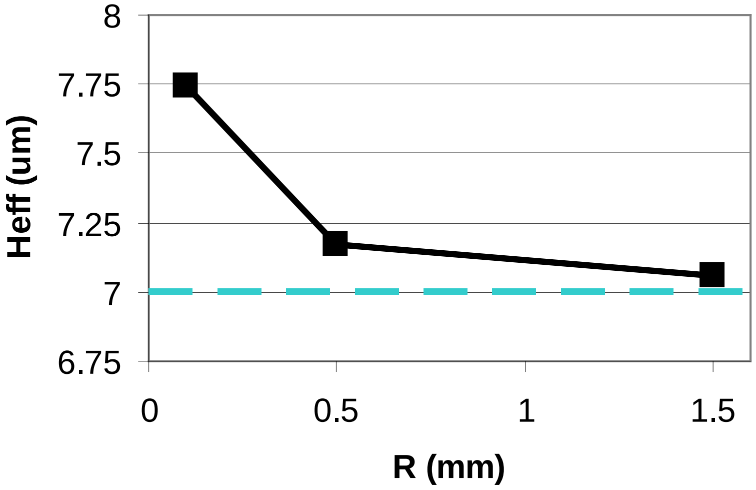
Microfluidic chip: inlet/outlet vias



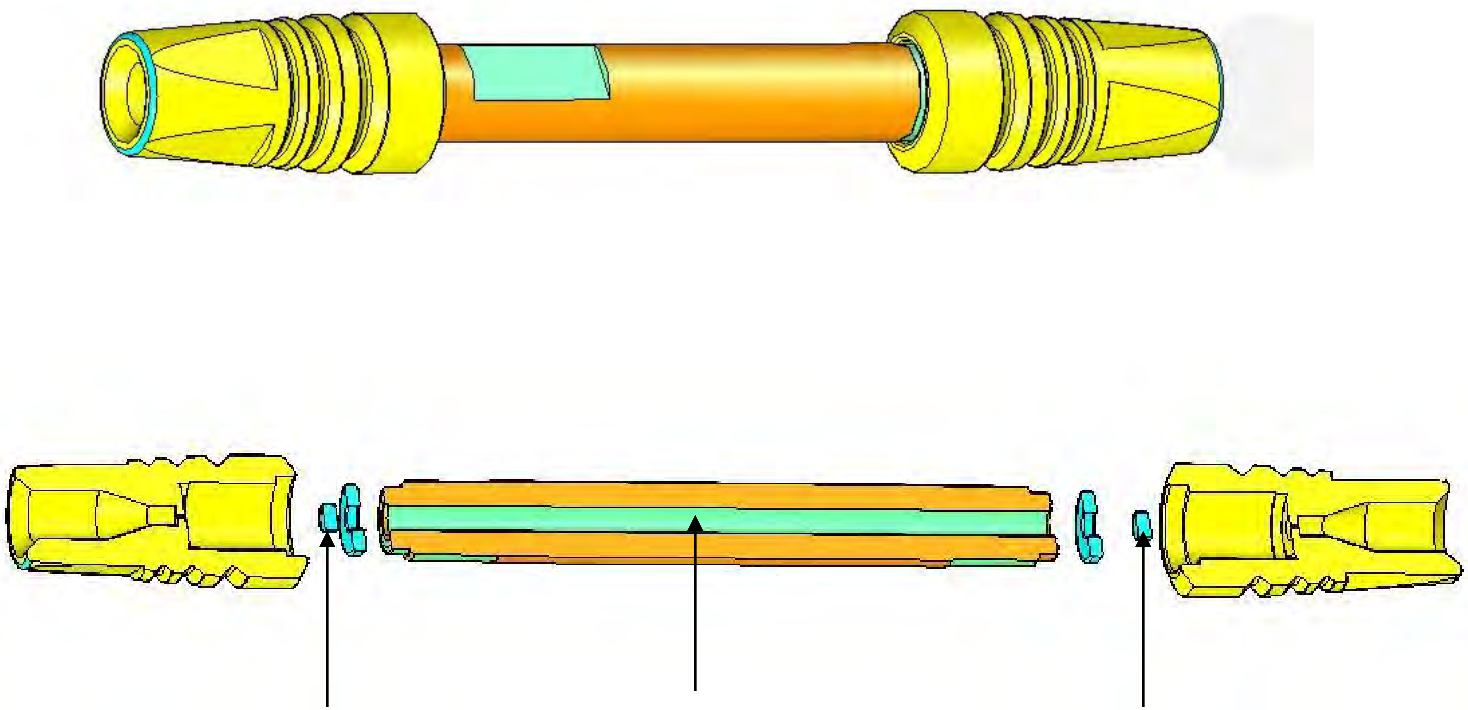


Microfluidic chip: bends





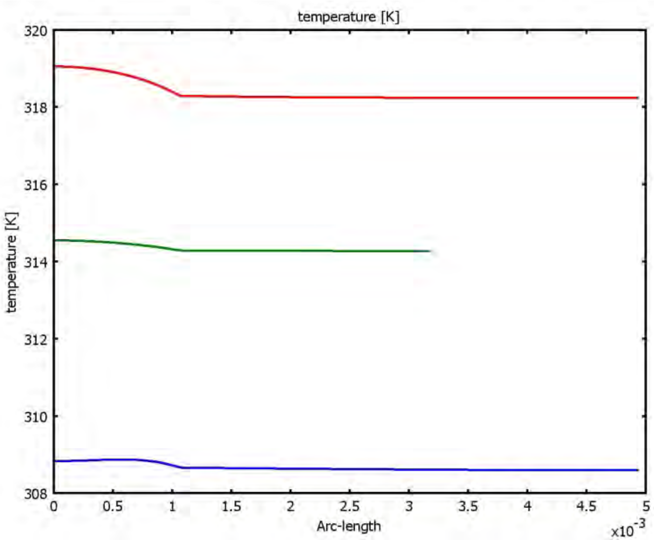
Thermal effects in 2.1 mm columns

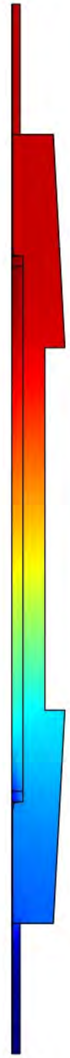


Temperature field

adiabatic BCs

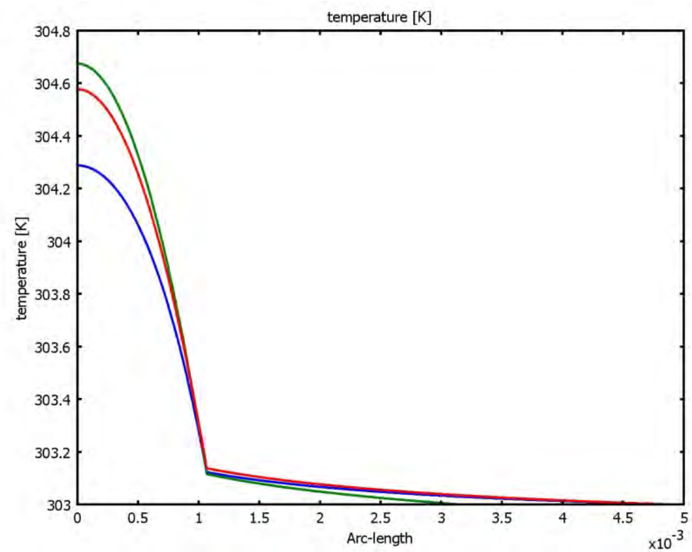
$\Delta T_{max} = 16.6$ K



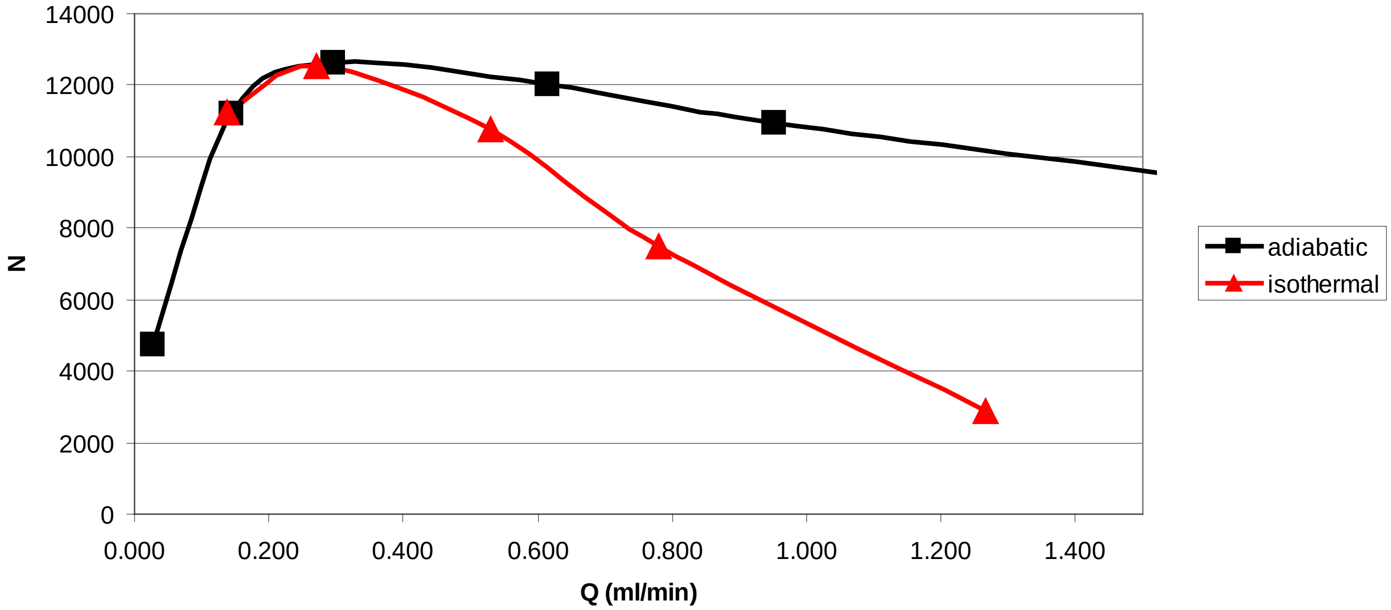


isothermal BCs

$\Delta T_{max} = 1.7$ K



Performance



- Heating and the temperature dependence of viscosity and diffusion coefficient can combine to create a significant drop of performance

Concluding remark

- Effect of artificial and numerical diffusion in convection-diffusion problems: