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Modeling Microfluidic Separations using Comsol Multiphysics

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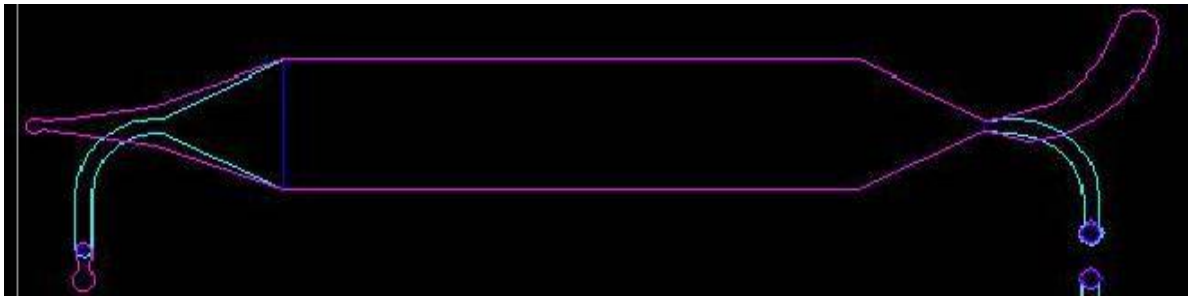
Laminar fluid diffusion interface channel (LFDI)



Courtesy of Micronics, Inc., Redmond, WA

Two fluids enter at the left, flow down a channel, are separated and two fluids leave at the right. If the fluids enter with different chemical compositions, diffusion and mixing takes place in the channel. The goal is to create two new fluid streams with desirable chemical compositions.

In the desired application, infrared spectroscopy will be used to identify creatinine (and metabolites) and the albumin (and proteins) need to be eliminated for good resolution.

Objectives

- Compare 2D with 3D models (use variance)
- Determine the impact of the inlet geometry
- Determine the impact of the outlet geometry
- Determine the enhancement factor

2D view

Parameters

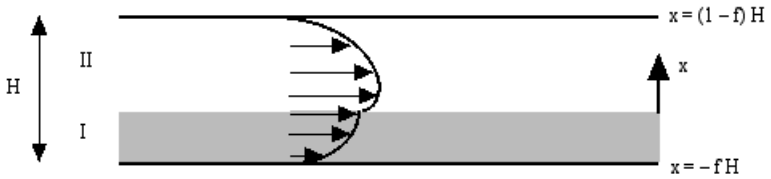
- Length = 22 mm
- Width = 4.5 mm
- Height = 330 μm
- Sample flow rate 1.02 μL/sec
- Receiver flow rate 1.84 μL/sec
- Viscosity 1 mPa s, 1.57 mPa s
- Density = 1 g/cm^3
- Diffusivity
  - 9.19 10-10 (creatinine, metabolite)
  - 6.7 10-11 (albumin, protein)

Reynolds number = 0.634

Peclet number = 689 (creatinine)

= 9460 (albumin)

Analytic Solution for Immiscible Fluids (Ind. Eng. Chem. Res.)

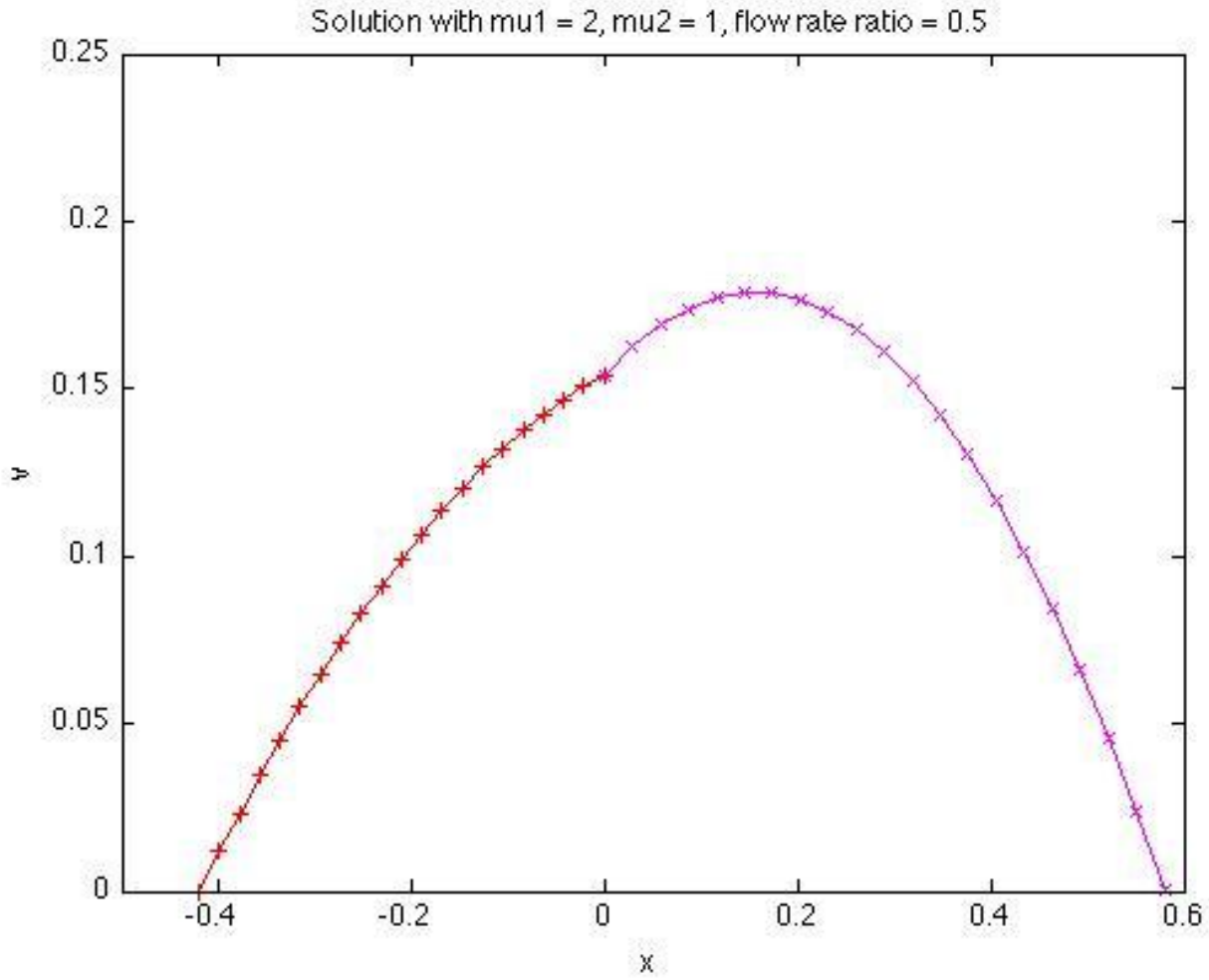


$$Q_1 = -\frac{\Delta p}{6\mu_1 L}(fH)^3 + \frac{C_1}{2\mu_1}(fH)^2 + C_2(fH)$$

$$Q_2 = -\frac{\Delta p H^3}{6\mu_2 L}(1-f)^3 - \frac{C_1 H^2}{2\mu_2}(1-f)^2 + C_2 H(1-f)$$

Given f, can calculate the flow rate ratio.
Given the flow rate ratio, need to solve for f numerically.

Flow Profiles for different viscosity ratios and different flow rate ratios



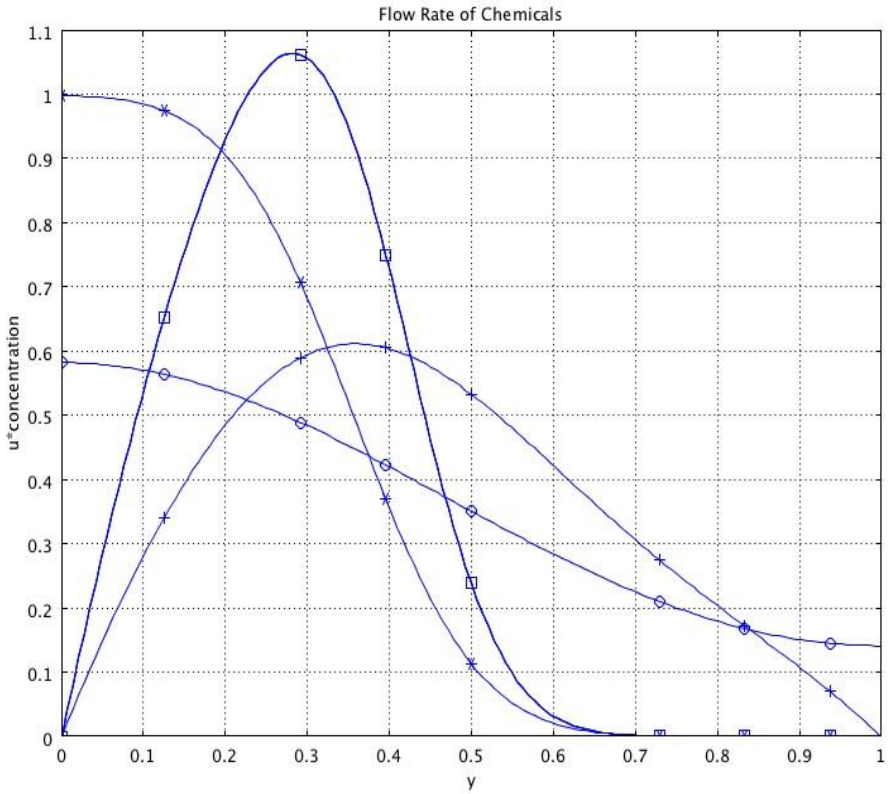
Performance Measures

$$\text{enhancement ratio} = \frac{\int_{productstream} c_{creatinine}\, u\, dA}{\int_{productstream} c_{albumin}\, u\, dA}$$

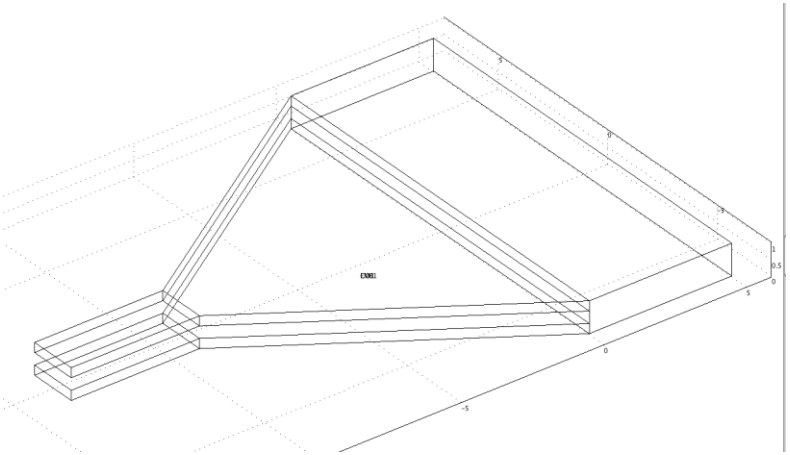
$$c_{\text{var}} = \frac{\int (c - c_{avg})^2 u dy}{\int u dy}$$

Diffusion Model

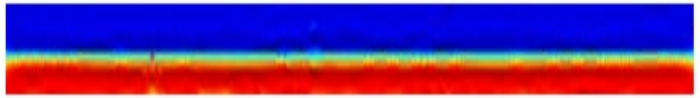
$$6y(1-y)\frac{\partial c}{\partial x} = \frac{1}{Pe}\frac{\partial^2 c}{\partial y^2} \qquad c(y,0) = 1,\ y \le 0.4032, 0 \text{ otherwise;}\ \frac{\partial c}{\partial y} = 0 \text{ at } y = 0, 1$$



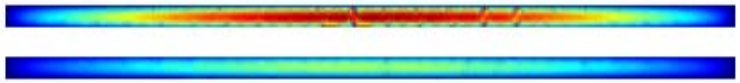
Inlet Expansion



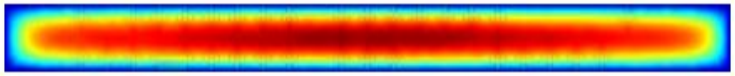
Flow: 906,794 dof; conc: 841,579 dof



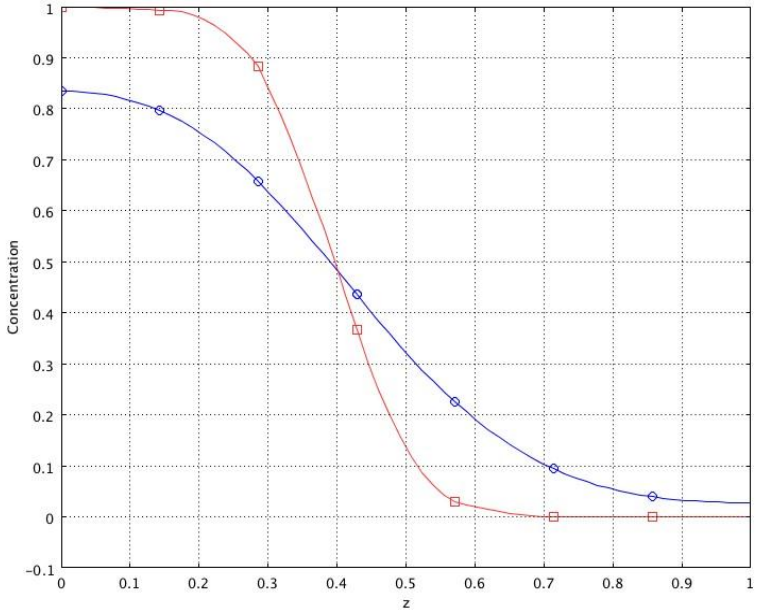
Concentration out of narrow neck (essentially two dimensional)



Velocity at end of expansion



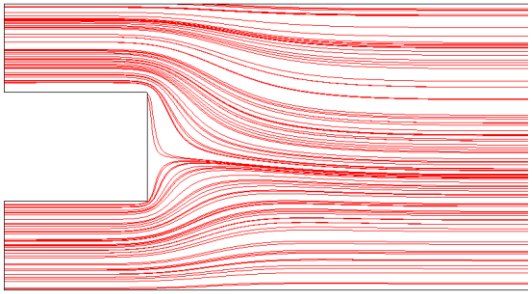
Velocity at end of 3D inlet



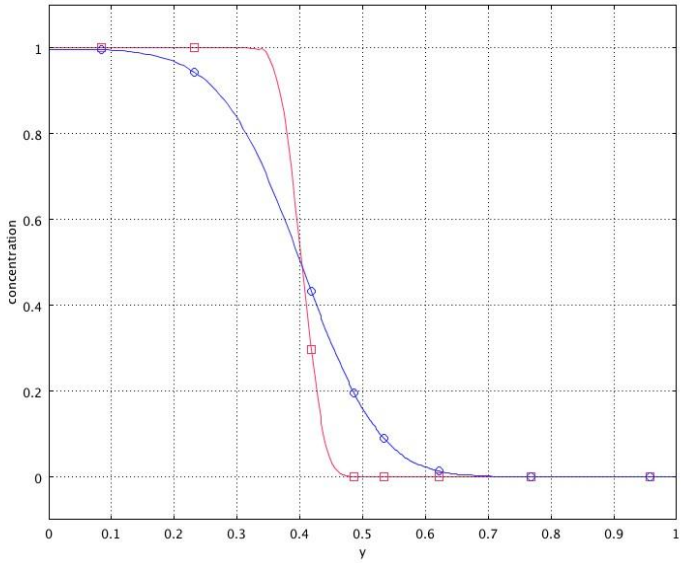
Concentration at exit (corner)

2D vs. 3D Comparisons

Converging flow at inlet.
Dividing streamline moves, but reaches asymptotic value quickly

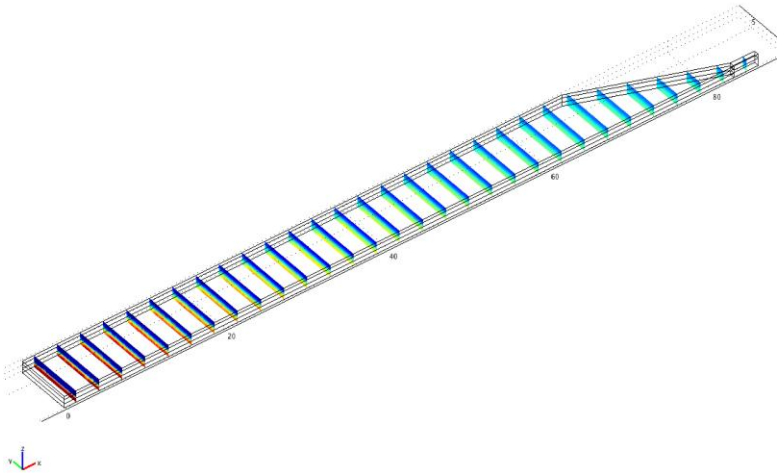


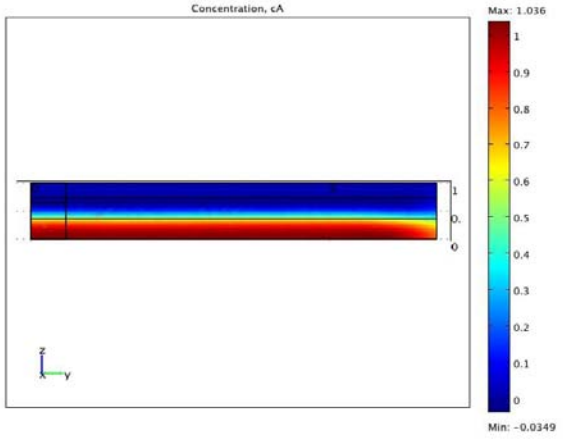
Average concentration = 0.3566 in all cases
Variances
Creatinine: 15% in 2D, 14% in 3D
Albumin: 21% in 2D, 20% in 3D



But albumin profiles are much steeper in 2D due to numerical diffusion in 3D simulations.

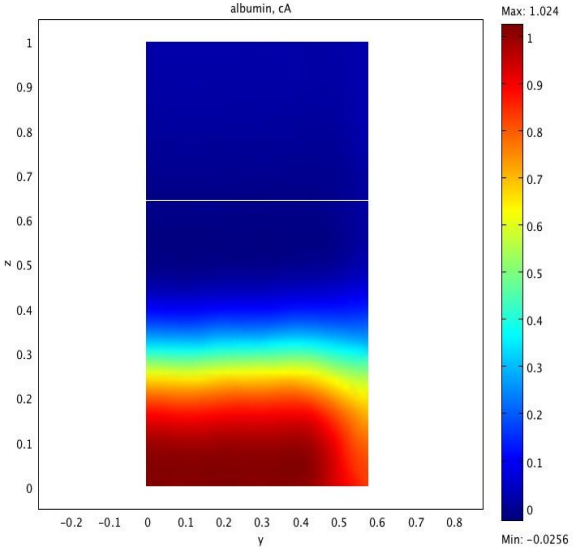
Exit region





Concentration of albumin
where channel starts to narrow

Amount going out the top:
Creatinine: 14% in 2D, 13% in 3D
Albumin: 0.055% in 2D, 0.28% in 3D

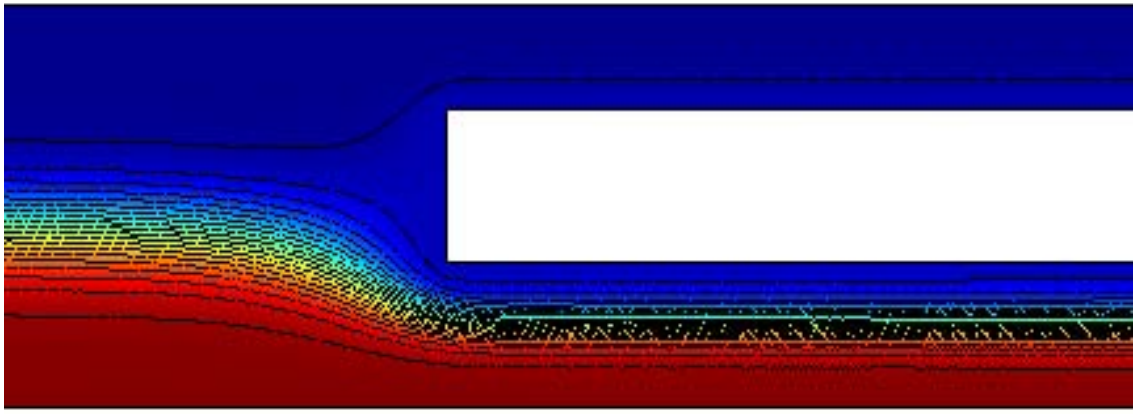


Concentration of albumin at exit.
Note the knife edge separation.

Flow: 376,934 dof (set for 18.5% out top);
creatinine: 287,446 dof;
albumin: 570,849 dof
Mass balances with 0.3%

Effect of Viscosity Ratio

$$\eta = 1 + 0.57 * cA$$



Relative viscosity: blue = 1, red = 1.57

Fraction of creatinine in upper stream is 24%; for albumin it is 0.58%.
Enhancement factor = 41.
With viscosity ratio = 1, enhancement factor = 66

Design Procedure

- For fixed flow rates of the two streams in, solve for *f*, the location of the dividing streamline.
- Estimate the thickness of the diffusion layer at a dimensionless distance *x* downstream from

$$\delta = \sqrt{12\,x/Pe}$$

Correct for the velocity at the dividing streamline being different from the average velocity.

$$\delta = \sqrt{12\,x/1.44 * Pe}$$

Place the divider at a distance *f* H + δ.

Conclusions

- The device can be modeled in Comsol Multiphysics.
- A 2D model suffices in most cases.
- A simple design procedure incorporates the major features.
- Large enhancement factors can be obtained with good design.
- Follow along my journey with 4.0 on www.ChemEComp.wordpress.com