

MODELING CONTROLLED RELEASE FROM CAVITIES IN MICROCHANNELS

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ABSTRACT

Computational simulations are presented of a novel method for controlling concentrations of solutes in microchannels. In this method, cavities in the walls of microchannels that contain chemicals are exposed to flowing solution, resulting in controlled dissolution of the solutes in question.

Keywords: Microfluidic, Transport

SIMULATION

Computational 2- and 3- D models were implemented using FEMLAB. The Navier-Stokes and convection-diffusion equations were used to simulate fluid motion and mass transport, respectively.

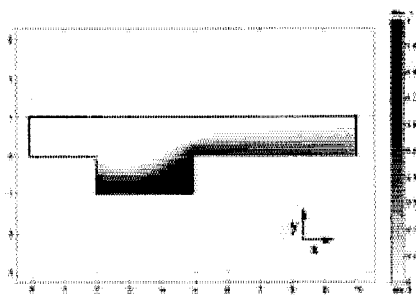


Figure 1. Result from 2-D model. The cavity was initially filled with a dextran solution.

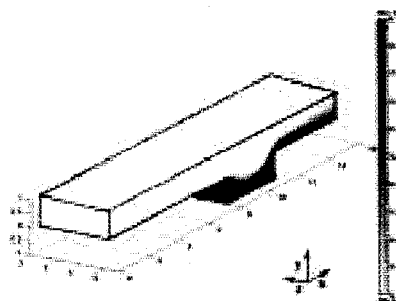


Figure 2. Result from 3-D model for a rectangular-shaped cavity.

The 2-D model (Figure 1) was created to examine the transport of concentrated solutions of dextran from cavities. Flow was simulated in the positive x-direction, and the inlet

(Figure 1) was given a parabolic velocity profile and a concentration of zero. The outlet was given straight-out and convective flux boundary conditions, while no slip and insulation boundary conditions were imposed at all other boundaries. The Pe number was 77.52, defined as the average velocity times a characteristic length of 100 μm divided by the diffusivity of a chemical in water. The Reynolds number was 3.75×10^{-4} , defined as the density times the average velocity times the characteristic length divided by the viscosity of pure water. The concentration of dextran was normalized to one, and an equation that describes the viscosity of dextran solutions as a function of concentration [1] was used to simulate the dynamic viscosity within the system. Time dependent simulations were performed for 30 model time units.

The 3-D model (Figure 2) was used to explore the steady-state transport of material from the bottom of rectangular- and cylindrical- shaped cavities. Re and Pe numbers, calculated as described above, were 10 and 100, respectively. Because of the symmetry of the system, half of each system was modeled (Figure 2) by giving the boundary in the x-y plane that intersects the cavity a slip condition. Flow was simulated in the positive x-direction. The velocity was normalized by the average inlet velocity, so that the model average velocity was 1.0, and all distances were normalized by 100 μm . All other boundary conditions were analogous to the 2-D model, except the boundaries representing the bottom of the cavities were set to a concentration of one.

RESULTS AND DISCUSSION

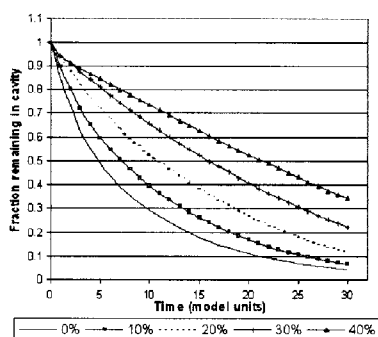


Figure 3. Dependence of the fractional of material released from the cavity on the concentration of dextran initially in the cavity. This is presumably due to the increasing viscosity of the material in the cavity at high concentrations.

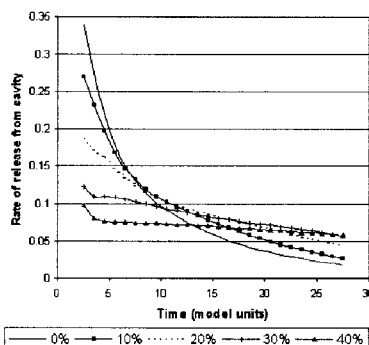


Figure 4. The corresponding rate of release from Figure 3. The simulated rate of release is nearly constant for long periods at high dextran concentrations. This begins to approximate the situation in which the material in the cavity is a solid.

Results from the 2-D model are shown (Figures 3 and 4). Concentration surface plots in the z-y plane at a distance of 5.5 units downstream from the center of a rectangular cavity (Figure 5) and a cylindrical cavity (Figure 6) obtained from the 3-D model (Figure 2) are presented.

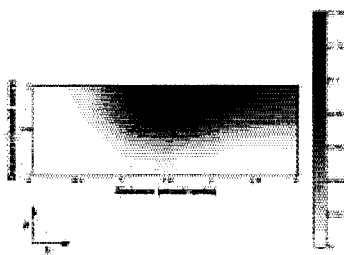


Figure 5. Concentration surface plot for rectangular cavity. Maximum concentrations were centered downstream from the corners of the cavity.

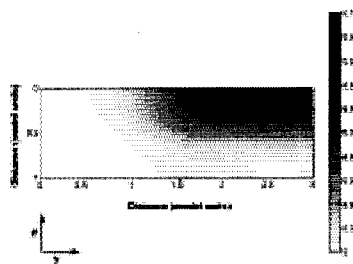


Figure 6. Concentration surface plot for cylindrical cavity. Maximum concentrations were located downstream from the center of the cavity.

CONCLUSIONS

Increasing the viscosity of the solution used to fill the cavity decreased and stabilized its rate of release from the cavity. The transport of a chemical released from rectangular- and cylindrical- shaped cavities resulted in different concentration distributions downstream from the cavity. These simulations suggest that the transport of a material from a cavity exposed to flow in a microchannel can be controlled using the viscosity of the material used to fill the cavity and its shape.

ACKNOWLEDGMENTS

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REFERENCES

- [1] Carrasco, F. & Chornet, E. A generalized correlation for the viscosity of dextrans in aqueous solutions as a function of temperature, concentration, and molecular weight at low shear rates. *Journal of Applied Polymer Science* 37, 2087-2098 (1989).