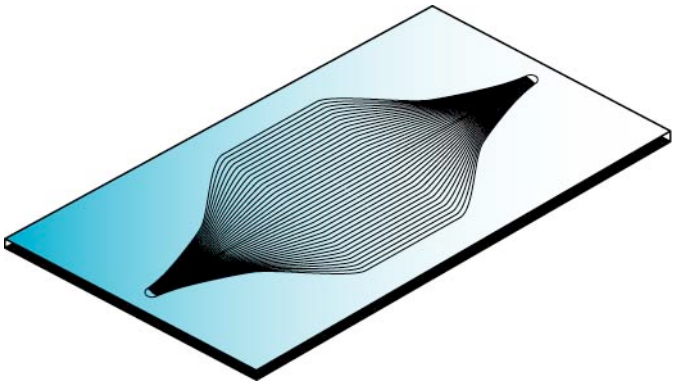
Maximum Adsorption in Microchannels



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Abstract

The purpose of the following project was to characterize the adsorption of the enzyme ADAMTS-13 and its antibody, anti-ADAMTS-13, onto a microchannel coated with the von Willebrand factor. COMSOL Multiphysics was used to develop both a one and three dimensional model of a channel with the following dimensions: 30 μm x 500 μm x 1 cm. The boundary condition of the walls were set such that anything that would diffuse to the walls would be adsorbed, thus giving a maximum adsorption of the enzyme and its antibody. With an approximation of 4 x 10^{-11} m^2/s for the diffusion coefficient of both molecules, it was found that for the given length of the channel above only 25% of the target molecules were removed from the fluid. In fact, in order to remove approximately 90% of the target molecules a minimum channel length of 28 cm is needed. A design summary is provided as Appendix II.

Introduction

ADAMTS-13 is an enzyme that cleaves the von Willebrand factor, which plays an important role in hemostasis. The antibody, anti-ADAMTS-13 attacks its counterpart. Unhealthy levels of either the enzyme or the antibody results in hemophilia or thrombosis respectively[1].

This report details results of the adsorption of ADAMTS-13 and its antibody onto the walls of a micro channel coated with vWF. The dimensions of the channel are as follows: 500 μm x 30 μm x 1 cm. The channel length can be adjusted (or multiple channels can be put in series) to accommodate for desired adsorption onto the walls.

Figure 1 depicts an illustration of the preliminary design of the blood chip that would be used to remove the target molecules.

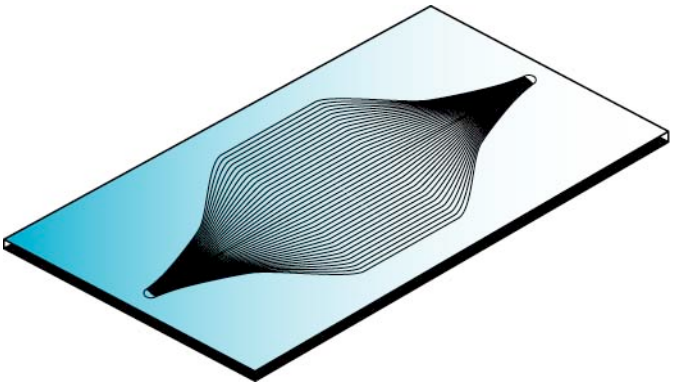

Figure 1: A drawing of the blood chip. The approximate dimensions of each channel are as follows 500 μm wide and 30 μm deep with each channel on the order of 1 cm in length.

Methods

In order to describe the concentration along the length of the channel the diffusion across the walls of the channel was solved.

$$u\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2} \qquad (1)$$

A 1D model was developed in COMSOL where the following one dimensional diffusion equation was used.

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad (2)$$

Substituting the definition of velocity, u, into the diffusion equation (1) we can see that the time component in (2) is analogous to the length of the channel, z.

$$t = \frac{z}{u} \qquad (3)$$

The boundary condition on the walls was defined by the following

$$c = 0 \qquad (4)$$

With this defined boundary condition, anything that diffuses to the wall will be adsorbed onto the surface. This assumption will give the maximum amount of the enzyme ADAMTS-13 and its antibody that can be adsorbed onto the walls.

In addition, the following assumptions were also made. The starting concentration of the target molecules in the fluid is .01 mol/m^3, the superficial velocity of the fluid in one channel is .056 m/s, the flow is fully developed, and the diffusion coefficient is approximately that of gamma globulin 4 x 10^{-11} m^2/s [2].

Results and Discussion

1-D Model

Preliminary results show that for nearly complete adsorption of the enzyme and antibody onto to the walls a very long channel length is required. We first consider the diffusion and adsorption along the shortest dimension of the micro channel, a depth of 30 μm. As shown in Figure 2, approximately only 25% of the target molecules are removed in a channel that is 1 cm in length. As a result of the large diffusion coefficient only small amounts of enzyme and its antibody diffuses to the walls and can be adsorbed. In fact, a channel length on the order 28 cm is required to remove approximately 90% of the enzyme and its antibody as seen in Figure 3.

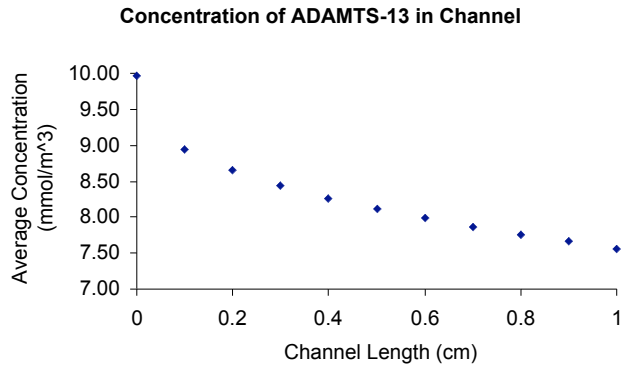

Figure 2: Concentration profile of ADAMTS-13 and its antibody along the length of the micro channel 1 cm in length.

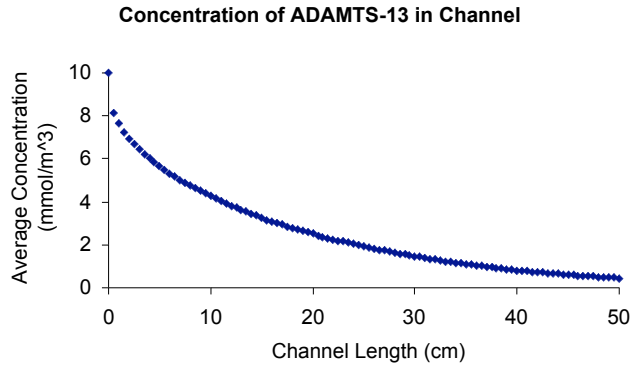

Figure 3: Concentration profile of ADAMTS-13 and its antibody along the length of the micro channel 50 cm in length.

Figure 4 is a plot of the diffusive flux at one of the two walls. The diffusive flux and adsorption along the walls is on the order of 10^{-7} mol/m^2-s. As stated before this is a result of the small diffusion coefficient.

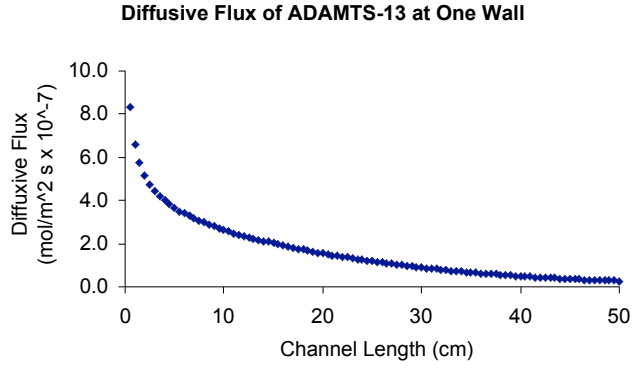

Figure 4: Diffusive flux of ADAMTS-13 and its antibody along one wall of the channel.

Diffusion along the width of the channel (500 μm) was also examined separately. The diffusion along this dimension was found to be negligible. As seen in Figure 5 only 4% of the target molecules diffuse and are adsorbed in this dimension.

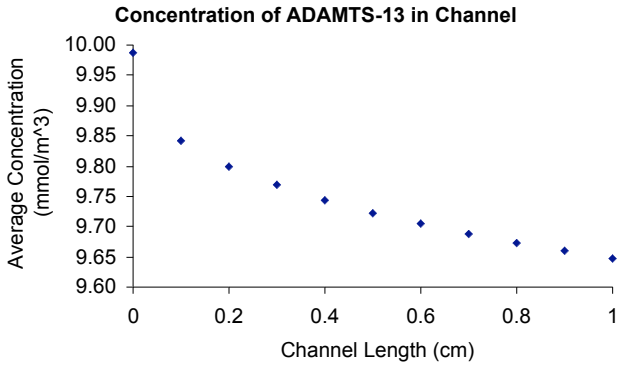

Figure 5: Concentration profile of ADAMTS-13 and its antibody along the length of a micro channel 1 cm in length.

Thus, the adsorption along the width of the channel can essentially be ignored. This can be further demonstrated by considering a three dimensional model of a channel that was developed. For a microchannel of the same length the concentration of the outlet was found to be 7.6 mmol/m^3. A difference of .7% from that found when considering just the adsorption along the depth of the channel, as seen in Figure 2.

The pressure drop across the channel was found to be 20 kPa/cm by modeling laminar flow through a narrow slit[3]. Given the same pressure drop across each channel the flow rate will indirectly proportional to the channel length, e.g. for a channel length of .5 cm the flow rate will be .112 m/s.

Conclusions

A minimum channel length of 28 cm is needed to remove approximately 90% of ADAMTS-13 and its anti-body from blood. These results provide a maximum limit to the amount of ADAMTS-13 and its antibody that are able to be adsorbed. For a more accurate description of adsorption of the molecules of interest experimental data should be obtained and or isotherms of similar enzymes.

References

[1] Motto, D G. "ADAMTS-13, VWF, Inflammation, and Thrombosis." Blood. 104. 1 (2004): 4.

[2] Porter, Mark C. Handbook of Industrial Membrane Technology. Park Ridge, N.J., U.S.A.: Noyes Publications, 1990. <http://www.knovel.com/knovel2/Toc.jsp?BookID=372>.

[3] Bird, R. Byron, Warren E. Stewart, and Edwin N. Lightfoot. Transport Phenomena. New York: J. Wiley, 2002.

Appendix I

Sample Calculation of Pressure Drop

The mass flow rate through a narrow slit is[3]:

$$w = \frac{2}{3}\frac{(\Delta P)D^3 W\rho}{\mu L}$$

where D is defined as half the depth, $15\times10^{-6}\,m$, W is $300\times10^{-6}\,m$, and L is $.01m$. Viscosity and density are the values stated in the Introduction.

$$(\Delta P) = \frac{3}{2}\frac{w\mu L}{\rho D^3 W} = \frac{3}{2}\frac{vA\mu L}{D^3 W} = \frac{3}{2}\frac{(.056m/s)(1.5\times10^{-8}m^2)(.0027Pa\cdot s)}{(15\times10^{-6}m)^3(500\times10^{-6}m)} = 20160Pa =$$

Data Exported from COMSOL

Channel Length	Average Concentration
cm	mmol/m^3
0.0	9.97
0.1	8.93
0.2	8.65
0.3	8.43
0.4	8.26
0.5	8.12
0.6	7.99
0.7	7.87
0.8	7.76
0.9	7.66
1.0	7.56

Channel Length	Average Concentration
cm	mmol/m^3
0.0	9.99
0.1	9.84
0.2	9.80
0.3	9.77
0.4	9.74
0.5	9.72
0.6	9.70
0.7	9.69
0.8	9.67
0.9	9.66
1.0	9.65

Table 1: Data for Figures 2 and Figures 5, left and right respectively.

Channel Length	Average Concentration	Channel Length	Average Concentration	Channel Length	Average Concentration
cm	mmol/m^3	cm	mmol/m^3	cm	mmol/m^3
0.0	10.0	17.0	2.93	34.0	1.16
0.5	8.15	17.5	2.86	34.5	1.13
1.0	7.62	18.0	2.79	35.0	1.10
1.5	7.25	18.5	2.72	35.5	1.07
2.0	6.95	19.0	2.64	36.0	1.03
2.5	6.67	19.5	2.57	36.5	1.00
3.0	6.43	20.0	2.50	37.0	0.97
3.5	6.21	20.5	2.43	37.5	0.95
4.0	6.02	21.0	2.37	38.0	0.92
4.5	5.84	21.5	2.31	38.5	0.89
5.0	5.66	22.0	2.25	39.0	0.86
5.5	5.47	22.5	2.20	39.5	0.84
6.0	5.32	23.0	2.14	40.0	0.81
6.5	5.17	23.5	2.08	40.5	0.79
7.0	5.02	24.0	2.03	41.0	0.77
7.5	4.86	24.5	1.97	41.5	0.74
8.0	4.74	25.0	1.92	42.0	0.72
8.5	4.62	25.5	1.86	42.5	0.70
9.0	4.51	26.0	1.81	43.0	0.68
9.5	4.39	26.5	1.77	43.5	0.66
10.0	4.27	27.0	1.72	44.0	0.64
10.5	4.15	27.5	1.68	44.5	0.62
11.0	4.03	28.0	1.64	45.0	0.60
11.5	3.91	28.5	1.60	45.5	0.58
12.0	3.81	29.0	1.55	46.0	0.56
12.5	3.72	29.5	1.51	46.5	0.55
13.0	3.63	30.0	1.47	47.0	0.53
13.5	3.53	30.5	1.42	47.5	0.51
14.0	3.44	31.0	1.38	48.0	0.5
14.5	3.35	31.5	1.34	48.5	0.5
15.0	3.25	32.0	1.31	49.0	0.5
15.5	3.16	32.5	1.27	49.5	0.5
16.0	3.08	33.0	1.23	50.0	0.4
16.5	3.00	33.5	1.20		

Table 2: Data for Figure 3.

Channel Length	Average Concentration	Channel Length	Average Concentration	Channel Length	Average Concentration
cm	mmol/m^3	cm	mmol/m^3	cm	mmol/m^3
0.0	1.9E+03	17.0	1.8E+00	34.0	7.0E-01
0.5	8.3E+00	17.5	1.8E+00	34.5	6.8E-01
1.0	6.6E+00	18.0	1.7E+00	35.0	6.6E-01
1.5	5.7E+00	18.5	1.7E+00	35.5	6.4E-01
2.0	5.1E+00	19.0	1.6E+00	36.0	6.2E-01
2.5	4.7E+00	19.5	1.6E+00	36.5	6.1E-01
3.0	4.4E+00	20.0	1.5E+00	37.0	5.9E-01
3.5	4.2E+00	20.5	1.5E+00	37.5	5.7E-01
4.0	4.0E+00	21.0	1.5E+00	38.0	5.5E-01
4.5	3.8E+00	21.5	1.4E+00	38.5	5.4E-01
5.0	3.7E+00	22.0	1.4E+00	39.0	5.2E-01
5.5	3.5E+00	22.5	1.4E+00	39.5	5.0E-01
6.0	3.4E+00	23.0	1.3E+00	40.0	4.9E-01
6.5	3.3E+00	23.5	1.3E+00	40.5	4.7E-01
7.0	3.2E+00	24.0	1.3E+00	41.0	4.6E-01
7.5	3.1E+00	24.5	1.2E+00	41.5	4.5E-01
8.0	3.0E+00	25.0	1.2E+00	42.0	4.3E-01
8.5	2.9E+00	25.5	1.2E+00	42.5	4.2E-01
9.0	2.8E+00	26.0	1.1E+00	43.0	4.1E-01
9.5	2.7E+00	26.5	1.1E+00	43.5	3.9E-01
10.0	2.6E+00	27.0	1.1E+00	44.0	3.8E-01
10.5	2.6E+00	27.5	1.0E+00	44.5	3.7E-01
11.0	2.5E+00	28.0	1.0E+00	45.0	3.6E-01
11.5	2.4E+00	28.5	9.7E-01	45.5	3.5E-01
12.0	2.3E+00	29.0	9.5E-01	46.0	3.4E-01
12.5	2.3E+00	29.5	9.2E-01	46.5	3.3E-01
13.0	2.2E+00	30.0	8.9E-01	47.0	3.2E-01
13.5	2.2E+00	30.5	8.7E-01	47.5	3.1E-01
14.0	2.1E+00	31.0	8.4E-01	48.0	3.0E-01
14.5	2.1E+00	31.5	8.2E-01	48.5	2.9E-01
15.0	2.0E+00	32.0	7.9E-01	49.0	2.8E-01
15.5	2.0E+00	32.5	7.7E-01	49.5	2.7E-01
16.0	1.9E+00	33.0	7.5E-01	50.0	2.6E-01
16.5	1.8E+00	33.5	7.3E-01		

Table 3: Data for Figure 4.

Appendix II

This appendix gives design equations and charts that enable one to design for maximum adsorption under conditions different from those in the report.

Calculation of Pressure Drop

As shown above, the total pressure drop is given by

$$\Delta p = \frac{3}{2}\frac{w\mu L}{\rho D^3 W}$$

where w = mass flow rate (kg/s)
μ = viscosity
L = channel length (m)
ρ = density (kg/m^3)
D = half-height (m)
W = width (m)

Using $w = \rho A\langle v\rangle$, $A = 2DW$, $Q = \langle v\rangle 2DW$

where A = cross sectional area (m^2)
Q = volumetric flow rate (m^3/s)
$\langle v\rangle = Q/A$ = average velocity (m/s)

we get

$$\Delta p = \frac{3}{2}\frac{Q\mu L}{D^3 W} \text{ or } \Delta p = \frac{3\langle v\rangle \mu L}{D^2}$$

Thus, the pressure drop in one channel is proportional to the velocity and pathlength and inversely proportional to the half-depth squared.

Calculation of concentration

The concentration is found by solving Eq. (1) above. The velocity is a quadratic function, symmetric about the centerline and zero on the boundaries.

$$u\ \frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2},\ c = 0 \text{ at } x = \pm D,\ c = 1 \text{ at } z = 0$$

The average concentration at any cross-section of the channel is

$$c_{avg} = \frac{\int_{-D}^{D} c(x,z)u(x)dx}{\int_{-D}^{D} u(x)dx}$$

A plot of the solution is in Figure II.1, which is similar to Figure 3.

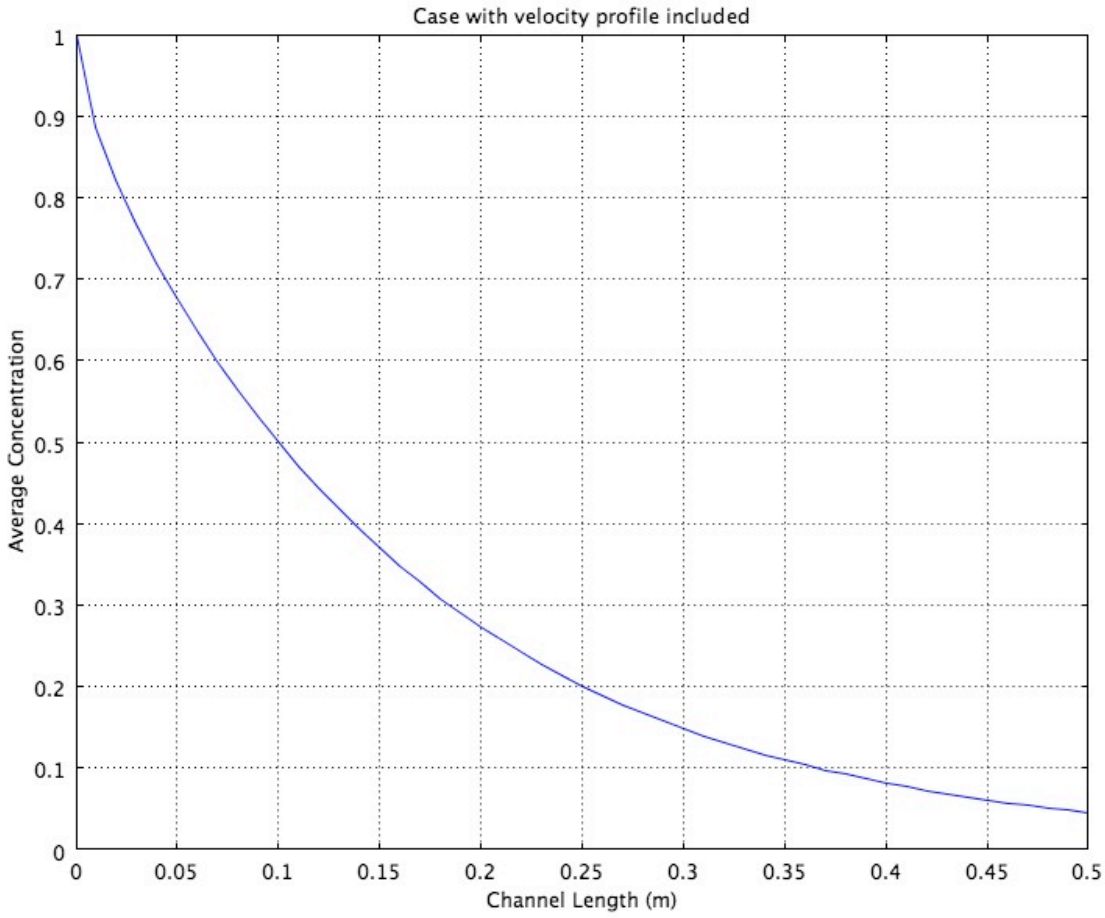

Figure II.1. Average concentration taking into account the parabolic velocity profile

It is also possible to solve this problem assuming a constant velocity profile, in which case one is solving

$$u_{avg}\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2},\ c = 0 \text{ at } x = \pm D,\ c = 1 \text{ at } z = 0$$

In this case the average concentration is given by

$$c_{avg} = \frac{\int_{-D}^{D} c(x,z)dx}{\int_{-D}^{D} dx}$$

The average concentration is now slightly different, as shown in Figure II.2.

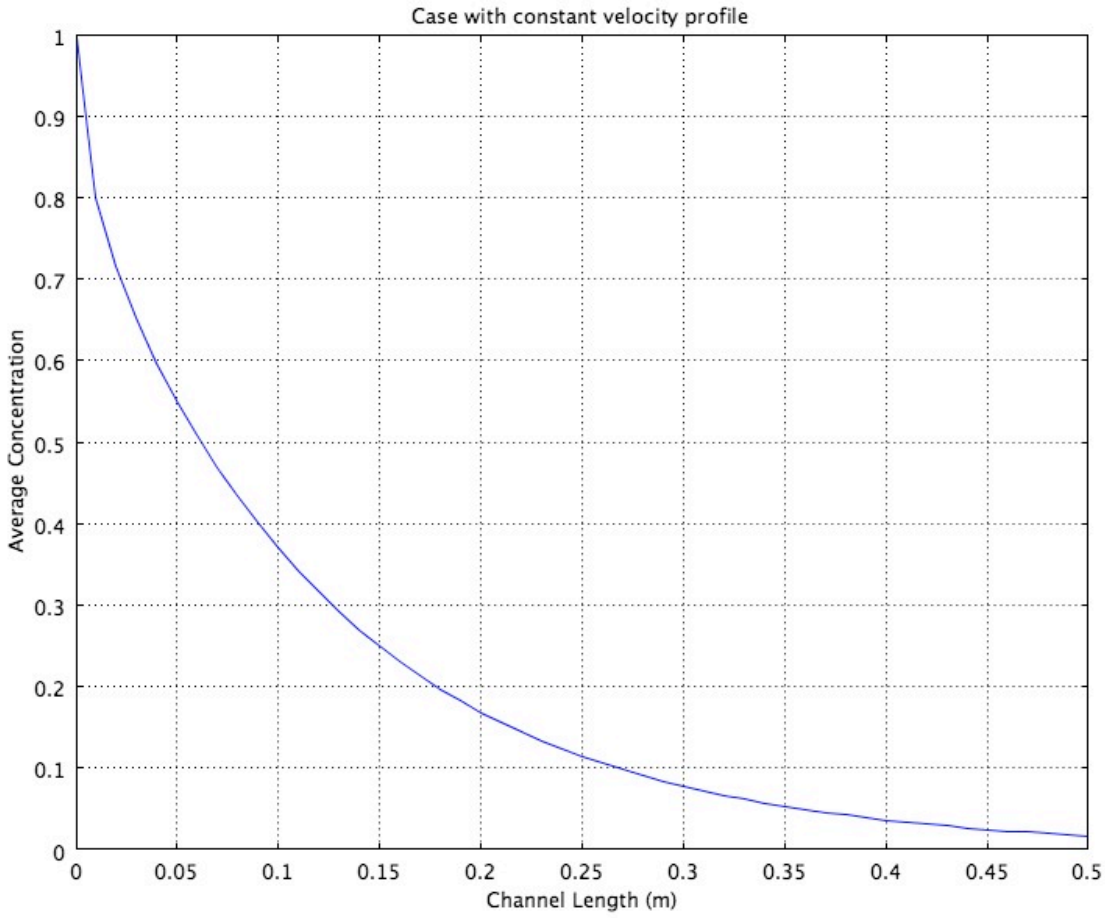

Figure II.2. Average concentration with a constant velocity profile

These two curves are compared in Figure II.3.

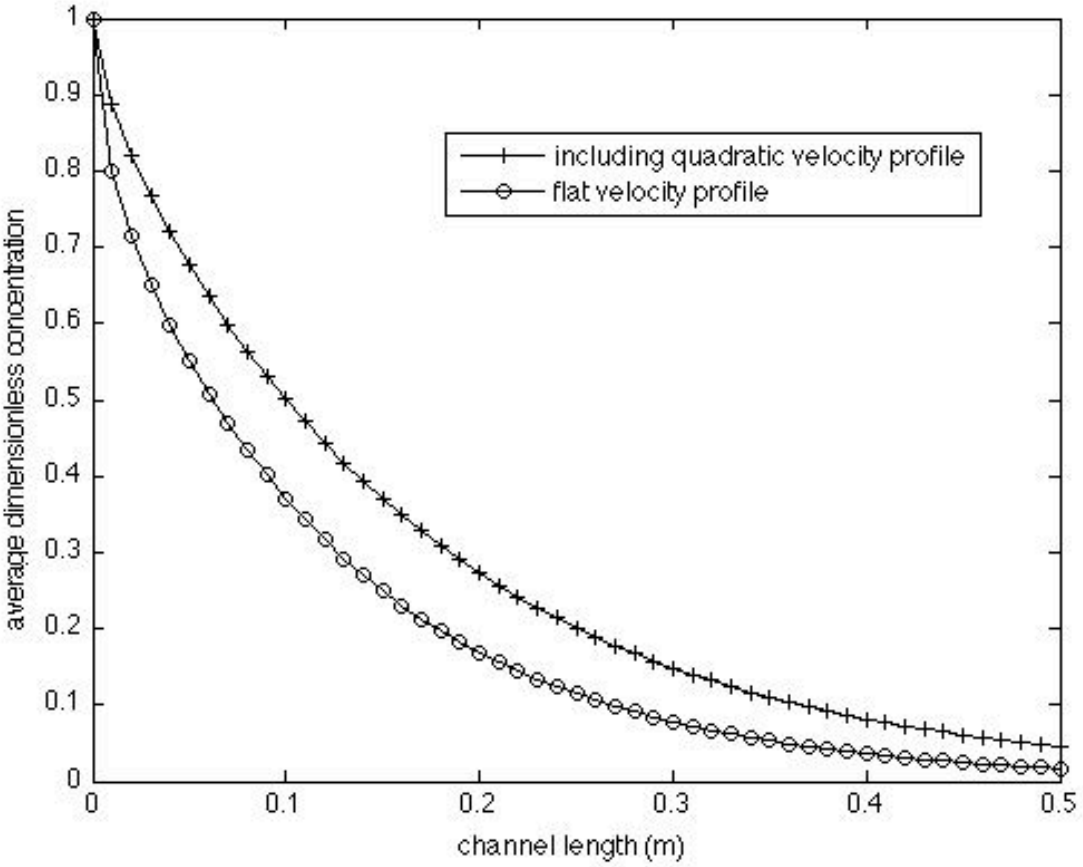

Figure II.3. Comparison of solutions with a parabolic or constant velocity profile

Universal curve

It is useful to have a universal curve so that the numerical calculations need not be done for each set of parameters. To do this, the equation is written in dimensionless form as follows. The distance is made dimensionless using the half-thickness, $x_s = D$, and the velocity is made dimensionless using the average velocity, $u_s = u_{avg}$. The length is defined as

$$z' = \frac{z}{z_s}$$

and the diffusion equation becomes

$$\frac{u' u_{avg}}{z_s} \frac{\partial c}{\partial z'} = \frac{D}{x_s^2} \frac{\partial^2 c}{\partial x'^2}$$

If we take $z_s = \frac{u_{avg} x_s^2}{D}$ (where here D is the diffusivity) the equation becomes

$$u' \frac{\partial c}{\partial z'} = \frac{\partial^2 c}{\partial x'^2}, c = 0 \text{ at } x' = \pm 1, c = 1 \text{ at } z' = 0, u' = 1.5(1 - x^2)$$

The solution to this equation with u'=1 can be compared with the solution for unsteady heat transfer (Ref. 3, p. 376) or similar solutions for mass transfer. When the velocity profile is quadratic, the average concentration is

$$c_{avg} = \frac{\int_{-1}^{1} 1.5(1 - x'^2) c(x', z') dx'}{\int_{-1}^{1} 1.5(1 - x'^2) dx'} = \int_{-1}^{1} 1.5(1 - x'^2) c(x', z') dx'$$

The solution in this form is a universal function that can be used for any thickness, velocity, diffusivity, or length.

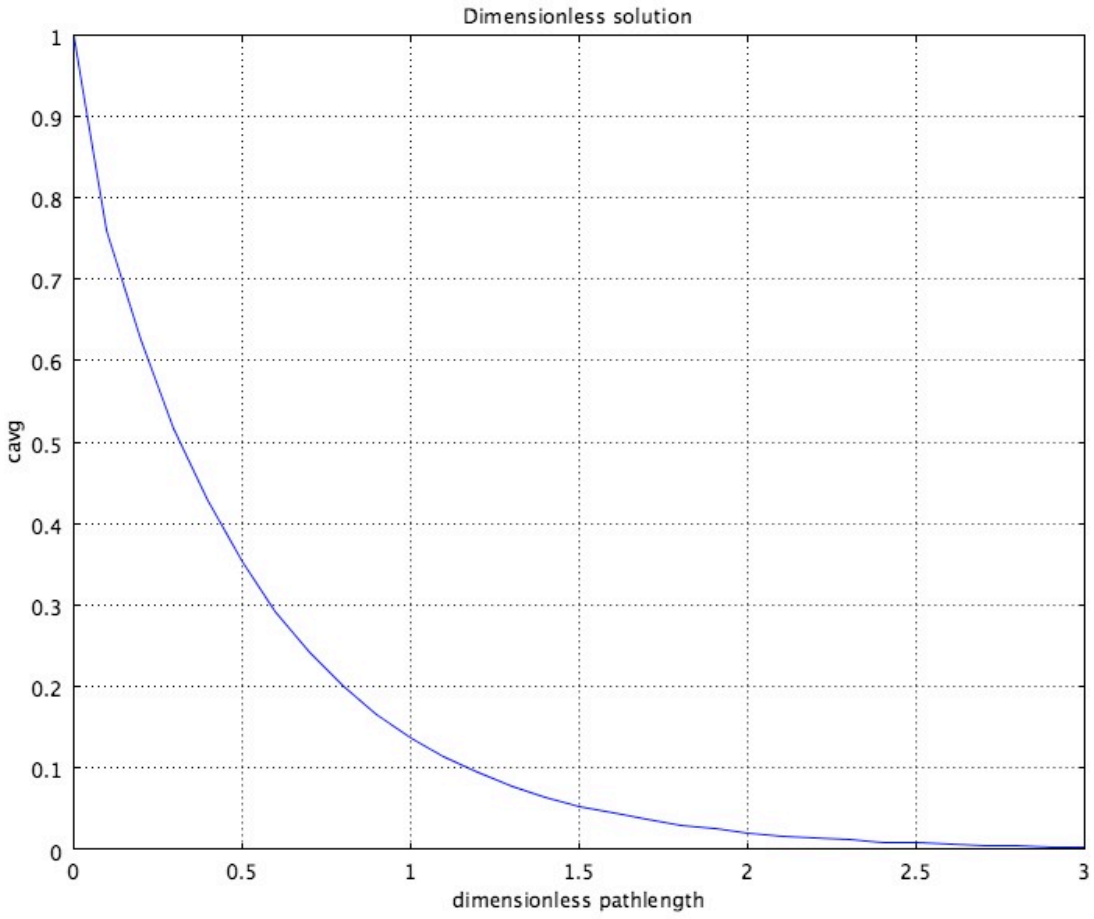

Figure II.4. Universal curve of average concentration versus dimensionless pathlength

One simply decides what fraction of the material you want absorbed (as an upper bound) and get the value of z' from Figure II.4. Then the length is given through the expression

$$z = z' z_s = z' \frac{u_{avg} x_s^2}{D}$$

For the case treated above z_s=0.315 m. Thus, , z'=1 in Figure II.4 corresponds to z_s=0.315 m in Figures II.1 and II.3.