Independent Project: H-Filter Purity and Collection Efficiency Characterization

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1 Introduction

Of the many ways to separate molecules, diffusion remains a popular choice. Diffusion works when the target particle has a diffusion coefficient different from the undesired particles. The two particles will then diffuse at different speeds. This difference in diffusion speeds can be leveraged. The "H-filter" is a commonly used filter that utilizes this difference in diffusion coefficients to separate particles. For an H-filter, the target particle must have a faster diffusion "speed" (larger diffusion coefficient) than the undesired particle. If this is not the case, then the highest purity that can be achieved is 50%, and an H-filter would not be a practical choice. An example of how how concentration profiles, for two different particles, change as time increases can be seen here: https://youtu.be/0wGytbAKjAk.

1.1 Background Information

In an H-filter, two microfluidic channels meet and become one with a width "w". The first channel contains a homogeneous solution of 2 particles, and the second contains only a buffer. They remain together for some length "L", and then separate again.



Figure 1: H-filter basic layout

1.1.1 Concentration and Purity

We want to optimize Purity and Collection efficiency (Cef). These functions are defined as followed:

$$Purity = \frac{\text{Count of desired particles at output}}{\text{total number of particles at output}}$$
(1)

$$Purity = \frac{\text{Count of desired particles at output}}{\text{count of desired particles} + \text{ count of undesired particles}}$$
(2)

$$Cef = \frac{\text{Count of desired particles at output}}{\text{count of desired particles at input}}$$
(3)

Let there be a concentration curve, C(x), for each particle in the (ENTIRE) channel:



Figure 2: 2 concentration profiles

The above concentration profiles show that the "blue" particles have diffused across the entire channel much more than the "red" particles. We can calculate each particle's count at the channel's output side by integrating the concentration curve along the width dimension (x) from the halfway point to the end (0.5 to 1, or w/2 to w).



Figure 3: Diagram of the Integral representing the count of particles at the output

For lack of a better letter, the count will be represented by A, because the count is the "A" rea or integral of concentration.

$$A(t) = \int_{w/2}^{w} C(x) \, dx$$
 (4)

If we let the desired particle be particle 1, then we can define purity with reference to particle 1.

$$Purity = \frac{\int_{w/2}^{w} C_1(x) \, dx}{\int_{w/2}^{w} C_1(x) \, dx + \int_{w/2}^{w} C_2(x) \, dx}$$
(5)

$$Purity = \frac{A_1}{A_2 + A_1} \tag{6}$$

We will define collection efficiency in a similar manner later, after introducing time dependence.

1.1.2 Flow rate, Flow velocity, and Dimensions

The flow rate, flow velocity, and dimensions are related to each other by the following equations.

Flow Rate = Cross Section Area
$$*$$
 Average Flow Velocity (7)

$$Q = A\bar{v}$$

$$A = width * height$$
(8)

$$A = wh \tag{9}$$

$$Q = wh\bar{v} \tag{10}$$

We can solve our Purity and Cef equations for only one 1-dimensional variable at a time (either length, width, or height). The most practical dimension to consider is width, which influences the diffusion rate and velocity. In order to solve for width, we can substitute the below expression for velocity.

$$\bar{v} = \frac{Q_{constant}}{w * h} \tag{11}$$

1.2 Goal

For this filter, we want to investigate the purity and collection efficiency (Cef) at the output. In particular, we want to investigate how the purity and collection efficiency changes in relation to channel geometry and flow speed. Our two main goals are:

- 1. Under dimensional constraints (length, height, width), and diffusion coefficient constraints (Dcoeff1, Dcoeff2) determine the flow velocity that would maximize purity for a given range of collection efficiency's.
- 2. Under flow rate constraints, and diffusion coefficient constraints, determine the ideal dimensions that would maximize purity for a given range of collection efficiency's. *Note:* that we are only able to let one dimension be unconstrained. In general the desired dimension to solve for is width, because it influences both the flow rate (Q) and flow velocity (v), and also influences the Purity and Collection Efficiency (Cef) functions. This is because our particles are diffusing along the width dimension.

2 Finding the Concentration Profile

The first step in solving for Purity and Cef is actually determining the concentration profiles. Let us make the following assumptions:

- 1. The flow velocity is constant and uniform throughout the entire channel and width of the channel. We will use the average flow velocity to represent flow velocity.
- 2. The sizes of the original two channels (before meeting) are identical, both having a width of w/2.
- 3. The diffusion coefficients of all particles remain constant.
- 4. diffusion only occurs in 1 direction (side to side); therefore, diffusion is not a prominent contributor or detractor to the particle speed in the flow direction.
- 5. Diffusion is not affected by velocity. In other words, the rate of diffusion is independent of the velocity. This assumption allows us to convert time and velocity using t = L/v.

We want to find the concentration profile as a function of x (location in the width dimension) at any point in the channel along the length dimension. An equivalent statement asks to find the concentration profile of a box of fluid with the square wave initial conditions after some time "t" has passed. This equivalency, along our assumptions, allows us to move from time to length using the fluid velocity as our conversion factor.

$$t = \frac{L}{v} \tag{1}$$

$$v = velocity \tag{2}$$

2.1 Governing Equation

Our governing equation is the differential equation of diffusion simplified into 1 dimension.

$$\frac{\delta C(x,t)}{\delta t} = D \frac{\delta^2 C(x,t)}{\delta x^2}$$
(3)

(4)

In order to solve this PDE, we need boundary conditions and an initial condition. The initial condition is the initial concentration gradient at time t = 0.

2.2 Boundary Condition

No diffusion should occur across the boundary (the walls) of the channel. This means the flux is 0 at the boundaries, x = 0 and x = w. This is true for all time $t \ge 0$. Mathematically we can state this as:

$$\frac{dC(x=0,t)}{dx} = 0\tag{5}$$

$$\frac{dC(x=w,t)}{dx} = 0 \tag{6}$$

(7)

2.3 Initial Condition

Our initial condition is represented by the initial concentration distribution. From our H-filter design, we can say that initially, the concentration is at some value C_i and is uniform throughout (0, w/2). Similarly, there are no particles in the other channel initially, so the concentration there is 0. We can normalize our curves by setting the initial concentration to 1. Our initial function is:

$$C(x, t = 0) = \begin{cases} 1 & \text{if } x \in [0, w/2] \\ 0 & \text{if } x \in [w/2, w] \end{cases}$$
(8)



Figure 4: Concentration profile at time = 0

2.4 Solving the PDE

Our governing equation differential equation is:

$$\frac{\delta C(x,t)}{\delta t} = D \frac{\delta^2 C(x,t)}{\delta x^2} \tag{10}$$

(11)

Note that Diffusion in 1 dimension, mathematically, is the same as equation for heat flow in 1 dimension, with the diffusion coefficient, D, replacing thermal conductivity k. This problem was famously solved by Fourier using his newly invented Fourier series. The solution to this differential equation with the given

boundary conditions is given by

$$C(x,t) = \sum_{n=0}^{\infty} A_n \cos(\frac{n\pi x}{w}) e^{-D\left(\frac{n\pi x}{w}\right)^2 t}$$
(12)

$$C(x,t) = A_0 + \sum_{n=1}^{\infty} A_n \cos(\frac{n\pi x}{w}) e^{-D(\frac{n\pi}{w})^2 t}$$
(13)

(14)

We can find these coefficient by applying our initial condition:

$$C_{t=0}(x) = C(x, t=0) = \begin{cases} 1 & \text{if } x \in [0, w/2] \\ 0 & \text{if } x \in [w/2, w] \end{cases}$$
(15)

(16)

Using this initial condition, we find that:

$$C_{t=0}(x) = A_0 + \sum_{n=1}^{\infty} A_n \cos(\frac{n\pi x}{w}) e^{-D\left(\frac{n\pi}{w}\right)^2 * 0}$$
(17)

$$C_{t=0}(x) = A_0 + \sum_{n=1}^{\infty} A_n \cos(\frac{n\pi x}{w})$$
(18)

(19)

In general, the Fourier expansion of a generic function f(x) with a period T is given by:

$$f(x) = A_0 + \sum_{n=1}^{\infty} (A_n \cos(n\omega x) + b_k \sin(n\omega x))$$
(20)

where
$$\omega = 2\pi/T$$
 (21)

(22)

And the coefficients for this generic function are:

$$A_0 = \frac{1}{T} \int_T f(x) dx \tag{23}$$

$$A_n = \frac{2}{T} \int_T f(x) \cos(n\omega x) dx$$
(24)

$$B_n = \frac{2}{T} \int_T f(x) \sin(n\omega x) dx$$
(25)

(26)

The period of the entire square wave is 2w (think -w to w), and we are investigating the part that is 0 to w. Therefore $\omega = 2\pi/(2w) = \pi/w$. We can quickly see for our function $C_{t=0}(x)$, the coefficients are:

$$A_0 = \frac{1}{w} \int_0^L C_{t=0}(x) \, dx \tag{27}$$

$$A_n = \frac{2}{w} \int_0^L C_{t=0}(x) \cos(\frac{n\pi x}{L}) \, dx$$
(28)

$$B_n = 0 \tag{29}$$

(30)

Note that our initial concentration function is 0 on the interval (w/2, w). Therefore, we can integrate everything from 0 to w/2 instead of 0 to w.

$$A_0 = \frac{1}{w} \int_0^{w/2} 1 \, dx \tag{31}$$

$$A_0 = \frac{1}{2} \tag{32}$$

$$A_{n} = \frac{2}{w} \int_{0}^{w/2} \cos(\frac{n\pi x}{w}) \, dx$$
(34)

$$A_n = \frac{2\sin(\frac{n\pi}{w})}{\pi n} \tag{35}$$

(36)

(38)

We can now assemble the solution to our PDE:

2.5 Solution

$$C(x, t, w, D) = \frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n} \right) \cos(\frac{n\pi x}{w}) e^{-D(\frac{n\pi}{w})^2 t}$$
(37)

We see that the concentration of an arbitrary particle in our H-filter is a function of:

- 1. x: the position along the width dimension
- 2. t: the time since diffusion has began. Time can be converted into velocity or width
- 3. w: the width of the channel
- 4. D: the diffusion coefficient

2.6 Compiling the Purity and Cef Equations

Using our concentration profile, we can now generate the functions for Purity and Collection efficiency by integration. The complete formulations for Purity and Cef are seen below:

2.6.1 Purity Equation

$$P_{D_1}(t, w, D_1, D_2) = \frac{A(t, w, D_1)}{A(t, w, D_1) + A(t, w, D_2)}$$
(39)

$$P_{D_1}(t, w, D_1, D_2) = \frac{\int_{w/2}^{w} \left[C(x, t, w, D_1) \right] dx}{\int_{w/2}^{w} \left[C(x, t, w, D_1) \right] dx + \int_{w/2}^{w} \left[C(x, t, w, D_2) \right] dx}$$
(40)

(41)

We can substitute in the equation for concentration profile:

$$P_{D_{1}} = \frac{\int_{w/2}^{w} \left[\frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n}\right) \cos(\frac{n\pi x}{w}) e^{-D_{1}\left(\frac{n\pi}{w}\right)^{2}t}\right] dx}{\int_{w/2}^{w} \left(\left[\frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n}\right) \cos(\frac{n\pi x}{w}) e^{-D_{1}\left(\frac{n\pi}{w}\right)^{2}t}\right] + \left[\frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n}\right) \cos(\frac{n\pi x}{w}) e^{-D_{2}\left(\frac{n\pi}{w}\right)^{2}t}\right]\right) dx}$$
(42)

Evaluating this integral:

$$P_{D_{1}} = \frac{\frac{w}{4} + \left(\frac{-2w}{\pi^{2}}\right) \sum_{n=1}^{\infty} \left(\frac{\sin^{2}(\frac{n\pi}{2})}{n^{2}}\right) \left(e^{-D_{1}\left(\frac{n\pi}{w}\right)^{2}t}\right)}{\frac{w}{4} + \left(\frac{-2w}{\pi^{2}}\right) \sum_{n=1}^{m} \left(\frac{\sin^{2}(\frac{n\pi}{2})}{n^{2}}\right) \left(e^{-D_{1}\left(\frac{n\pi}{w}\right)^{2}t}\right) + \frac{w}{4} + \left(\frac{-2w}{\pi^{2}}\right) \sum_{n=1}^{\infty} \left(\frac{\sin^{2}(\frac{n\pi}{w})^{2}t}{n^{2}}\right) \left(e^{-D_{2}\left(\frac{n\pi}{w}\right)^{2}t}\right)$$
(43)

Simplifying:

$$P_{D_1}(t, w, D_1, D_2) = \frac{\frac{w}{4} + \left(\frac{-2w}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\left(\frac{\sin^2(\frac{n\pi}{2})}{n^2}\right) \left(e^{-D_1\left(\frac{n\pi}{w}\right)^2 t}\right) \right]}{\frac{w}{2} + \left(\frac{-2w}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\left(\frac{\sin^2(\frac{n\pi}{2})}{n^2}\right) \left(e^{-D_1\left(\frac{n\pi}{w}\right)^2 t} + e^{-D_2\left(\frac{n\pi}{w}\right)^2 t}\right) \right]}$$
(44)

This is our expression for Purity. In general, we will use numerical methods to find solutions.

Note: If we have different initial concentrations, then Purity would also be a function of the initial concentration of each particle.

We can write the Purity function in three (3) ways: in terms of time, velocity, or width. We can substitute t = L/v and then solve for velocity, or substitute $t = \frac{whL}{Q}$ and solve for width. These formulations can be more physically useful then solving for time.

$$P_{D_1}(t, w, D_1, D_2) = \frac{A(t, w, D_1)}{A(t, w, D_1) + A(t, w, D_2)}$$
(46)

$$in \, length \, / \, velocity : t = L/v \tag{47}$$

$$P_{D_1}(t, w, D_1, D_2) = P_{D_1}(L/v, w, D_1, D_2) = \frac{A(L/v, w, D_1)}{A(L/v, w, D_1) + A(L/v, w, D_2)}$$
(48)

$$in \ width: v = \frac{Q}{wh} \longrightarrow t = \frac{whL}{Q}$$
(49)

$$P_{D_1}(t, w, D_1, D_2) = P_{D_1}(\frac{whL}{Q}, w, D_1, D_2) = \frac{A(\frac{whL}{Q}, w, D_1)}{A(\frac{whL}{Q}, w, D_1) + A(\frac{whL}{Q}, w, D_2)}$$
(50)

2.6.2 Collection Efficiency Equation

Collection efficiency is defined as the number of particles at the output divided by the number of particles at the input. The number of particles at the input, by definition, is the integral of the concentration over the input (from 0 to w/2).

$$Cef(t, w, D) = \frac{A(t, w, D)}{A(t = 0, w, D)}$$
 (51)

(52)

(45)

Because the integral in the denominator no longer has time dependence (t always equals 0), we are going to relabel it. Let:

$$Cef(t, w, D) = \frac{A(t, w, D)}{A_{start}(w, D)}$$
(53)

Now, calculating Astart

$$A_{start}(w,D) = \int_0^{w/2} C(x,t=0,w,D)dx$$
(54)

$$A_{start}(w,D) = \int_0^{w/2} \frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n}\right) \cos(\frac{n\pi x}{w}) e^{-D(\frac{n\pi}{w})^2 * 0} dx$$
(55)

$$A_{start}(w,D) = \int_0^{w/2} \frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n}\right) \cos(\frac{n\pi x}{w}) dx$$
(56)

We see that A_{start} is also not a function of the diffusion coefficient for this particle. This is because we are at t = 0, so no diffusion is happening.

$$A_{start}(w) = \int_0^{w/2} \frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{2\sin(\frac{n\pi}{w})}{\pi n} \right) \cos(\frac{n\pi x}{w}) dx$$
(57)

$$A_{start}(w) = \frac{w}{4} + \left(\frac{2w}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\frac{\sin^2(\frac{\pi n}{2})}{n^2}\right]$$
(58)

We have now evaluated the denominator of Cef, and the numerator, A(t, w, D), was already evaluated when calculating Purity. Our Cef Function is therefore:

$$Cef(t, w, D) = \frac{\frac{w}{4} + \left(\frac{-2w}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\left(\frac{\sin^2(\frac{n\pi}{2})}{n^2}\right) \left(e^{-D_1\left(\frac{n\pi}{w}\right)^2 t}\right) \right]}{\frac{w}{4} + \left(\frac{2w}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\frac{\sin^2(\frac{\pi n}{2})}{n^2}\right]}$$
(59)

¹ This is our expression for Collection Efficiency. In general, we will use numerical methods to find solutions.

Note: If we have different initial concentration, then Cef would also be a function of the initial concentration of our target particle.

We can also substitute Length/velocity and $\frac{whL}{Q}$ for t in Cef just as we did for Purity. This gives us three equivalent forms of Cef to work with:

. /

in time:
$$(60)$$

$$Cef(t, w, D) = \frac{A(t, w, D)}{A_{start}(w, D)}$$
(61)

$$in \, length \, / \, velocity : t = L/v \tag{62}$$

D)

$$Cef(t, w, D) = Cef(L/v, w, D) = \frac{A(L/v, w, D)}{A_{start}(w, D)}$$
(63)

$$in \ width: v = \frac{Q}{wh} \longrightarrow t = \frac{whL}{Q}$$
(64)

$$Cef(t, w, D) = Cef(\frac{whL}{Q}, w, D) = \frac{A(\frac{whL}{Q}, w, D)}{A_{start}(w, D)}$$
(65)

¹The sum in the denominator converges to approximately 1.2337

$$\sum_{n=1}^{\infty} \left[\frac{\sin^2(\frac{\pi n}{2})}{n^2} \right] \approx 1.2337$$

2.7 Matlab

We represent these equations in Matlab with the following:

```
6
         %%
 7
 8
         % Setting up functions:
9
         % The sum term
                                      s(n)
                                                   ,the fundemental solution
10
         %
                                                   ,n is the number of terms being
11
                                                  summed
         %
12
         % Concentration:
                                      C(y,t,w,D)
13
         % Area aka count:
                                      A(t,w,D)
14
         % Purity:
                                      Purity(t,w,D1,D2)
15
         % Collection Efficiency:
                                      Cef(t,w,D)
                                      Astart(w,D) , for use in collection effeciency
16
         % Astart
17
18
         syms n D D1 D2 w x t L v
19
20
21
22
         s(n) = ((2*sin(pi*n/2))/(pi*n))*cos(n*pi*(x)/w)*exp(-D*t*(n*pi/w)^2);
23
24
25
26
         C(x,t,w,D) = 1/2 + symsum(s(n),n,1,1000); % note that this function can take
27
                                                   % awhile to run due to summing n
28
                                                   % terms. Reduce term number to
29
                                                   % decrease run time.
30
31
         A(t,w,D) = int(C(x,t,w,D),x,w/2,w);
32
         Astart(w,D) = int(C(x,0,w,D),x,0,w/2);
33
         Cef(t,w,D) = A(t,w,D)/Astart(w,D);
34
35
         Purity(t,w,D1,D2) = (A(t,w,D1))./ (A(t,w,D1) + A(t,w,D2));
36
```

Figure 5: Matlab

3 Extremes

What is the trend for purity and collection efficiency at the extremes?

3.0.1 Time

As time approaches zero, the amount of time available for diffusion approaches zero. Therefore, the amount of both particles that can diffuse converges as time approaches zero, and therefore, the purity becomes 50% as time approaches zero.

$$\lim_{t \to 0} P = 0.5 \tag{66}$$

$$\lim_{t \to 0} Cef = 0 \tag{67}$$

As time approaches infinity, purity will also approach 50%, as both particles will have sufficient time

to diffuse across the channel fully. Furthermore, because all particles are fully diffused, the collection efficiency will also approach 50%.

$$\lim_{t \to \infty} P = 0.5 \tag{68}$$

$$\lim_{t \to \infty} Cef = 0.5 \tag{69}$$

3.0.2 Velocity

Velocity and time have an inverse relationship:

$$t = L\frac{1}{\nu} \tag{70}$$

A low velocity will let diffusion occur for a long time before the particles reach the end of the channel (i.e., the output), and a high velocity allows for a small amount of time for diffusion to occur.

As velocity tends to infinity, time will tend to 0. Therefore, As velocity tends to infinity, Purity will tend to 50%, and Cef will tend to 50%.

$$\lim_{v \to \infty} P = 0.5 \tag{71}$$

$$\lim_{v \to \infty} Cef = 0 \tag{72}$$

As velocity tends to zero, time will tend to infinity. Therefore, as velocity tends to 0, Purity will tend towards 50% and Cef will tend towards 50%.

$$\lim_{v \to 0} P = 0.5 \tag{73}$$

$$\lim_{v \to 0} Cef = 0.5 \tag{74}$$



Figure 6: Graphs of Purity and Cef against Time and Velocity

3.0.3 Width

For a constant flow rate Q, we use these equations:

$$P_{D_1}(\frac{whL}{Q}, w, D_1, D_2) = \frac{A(\frac{whL}{Q}, w, D_1)}{A(\frac{whL}{Q}, w, D_1) + A(\frac{whL}{Q}, w, D_2)}$$
(75)

$$Cef(\frac{whL}{Q}, w, D) = \frac{A(\frac{whL}{Q}, w, D)}{A_{start}(w, D)}$$
(76)

We can see that width is an input twice. Width now controls the flow velocity by changing the cross-section dimensions, and width also controls the actual width of the channel, which directly influences how long it takes for diffusion to occur across the channel. Width and time are directly proportional, while velocity and width are inversely proportional.

$$t = \frac{whL}{Q} \tag{77}$$

$$v = \frac{Q}{wh} \tag{78}$$

When the width approaches zero, the flow velocity approaches infinity (assuming a constant flow rate). This means that the particles will fly through the channel to the output without sufficient time to diffuse across (as discussed earlier). However, we are also directly changing the channel width and making it smaller, and therefore complete diffusion (i.e., reaching a Cef of 0.5) requires less time. These two effects compete, but the decrease in channel width wins out over the increase in velocity. As width tends to 0, collection efficiency tends to 50%. For the same reason, Purity also approaches 50%.

$$\lim_{w \to 0} P = 0.5 \tag{79}$$

$$\lim_{w \to 0} Cef = 0.5 \tag{80}$$

When the channel width approaches infinity, the amount of time *required* to diffuse throughout the channel approaches infinity, and the flow velocity approaches zero. Once again, these two effects compete. A low flow velocity will give more time for complete diffusion, but a large width means it takes longer. In general, the dominant effect is the direct increase in width and its corresponding effect of increasing the time requirement for complete diffusion and, therefore, decreasing Cef.

$$\lim_{w \to \infty} P = 0.5 \tag{81}$$

$$\lim_{w \to \infty} Cef = 0 \tag{82}$$



Figure 7: Graphs of Purity and Cef against Width. 1000 sum terms, 5300 data points total

4 Other problem types

4.1 Initial Concentrations Not Equal

How do we approach these problems if the initial concentrations of each particles are not equal to each other? We can solve the diffusion PDE for each particle and it's initial concentration conditions, and then use each particles concentration profiles for the purity and collection efficiency equations.

4.2 Constraining or optimizing Run-time

Similar to how we constrained or tried to solve for velocity and width, it is also possible to solve for run-time or solve for other values (ie, dimensions) if we constrain runtime. Run-time is the time it takes for the filter to produce an output. In other words, the time it takes for a particle to go from the input to the output of the filter. If we are trying to sort a large amount of particles, run-time may be of particular concern.

5 Results

Let's solve two example problems that each align with one of our goals. The first example problem is taken from BIOE 174, the second I generated myself.

5.1 Example Problem 1

We want to separate 15 nm diameter polystyrene beads ($D = 10^{-12}m^2/s$) from E.coli (*Decoli* = $10^{-14}m^2/s$) using a microfluidic H-filter. H-filter has channel height, h = 10 micrometers; width, w = 100 micrometers and length, L = 1 cm.

- 1. What is the approximate particle speed and the flow rate that is needed for separation of beads with purity of at least 80% (assume that the input concentrations are approximately equal for the beads and E.coli)?
- 2. What is the Collection efficiency at this speed?

We are given

$$Dcoeff1 = 10^{-12}$$
 (1)

$$Dcoeff2 = 10^{-14}$$
 (2)

$$L = 0.01m \tag{3}$$

$$h = 10 * 10^{-6} \tag{4}$$

$$w = 100 * 10^{-6} \tag{5}$$

$$P_{desired} = 0.8 \tag{6}$$

$$C_1|_{t=0} = C_2|_{t=0} \tag{7}$$

We could approach this problem in the following (although there are likely other ways):

1. Solve for the "time value" by setting the purity function equal to 0.8. This time value can easily be converted into a velocity using v = L/t. Now we have a velocity (and we can quickly find a flow rate using Q = Av).

- 2. Use the time value to calculate a Cef using the Cef function. This both gives us the answer to part b, and validates our solution.
- 3. It is highly encouraged to graph our solution. Sometimes we can actually a achieve a better combination of Purity and Cef, and graphing will validate our answers.



Figure 8: Matlab





Figure 9: Graph of Purity and Cef, in log and linear scales vs Velocity. 1000 sum terms, 3000 data points

Highlighted are the solution points, and also another set of points. This second set, at a velocity of 2e - 6, shows how we can sometimes greatly improve purity (and decrease runtime by increasing velocity), while only sacrificing a very small amount of collection efficiency.

5.2 Example Problem 2

Let us take the same problem, but instead of being given the width we are given the flow rate and want to solve for width. In order to solve the problem, we must specify a value for the length and height dimensions. For this problem, our values are:

Dcoeff1 =
$$10^{-12}$$
 (8)

Dcoeff2 =
$$10^{-14}$$
 (9)

$$L = 0.01m\tag{10}$$

$$h = 10^{-5} \tag{11}$$

$$Q = 5.3mm^3/s = 5.3 * 10^{-7}m^3/s \tag{12}$$

We can solve this problem 2 ways. We can find the optimal width to maximize Purity, or we can find the optimal width to maximize Collection Efficiency. I would argue the best approach to this problem, from the design perspective, is a graphical approach. Similar to example 1, it is easy to graph how Purity and Cef change with Width, and then we can pick what combination of Purity and Collection efficiency we want. Before graphing, it is useful to solve for a width with both an ideal Cef of 0.49 and a good purity of 0.8-0.9. This gives us an idea of what range of widths to graph on (if we don't already have a range of suitable widths in mind).



Figure 10: Matlab

Graphing our functions:



Figure 11: Graph of Purity and Cef vs Width, in log scale 1000 sum terms, 2100 data points

If we were to build this H-filter, we would likely want to choose a width around $10^{-2}m$.

Note: small tip: I have found it is best to solve with the condition of Cef() = 0.49. This gives you a value (of velocity, or width, or whatever you are solving for) that lies on the curved section of the graph. If you solve for Cef = 0.5 you are likely to end up on the flat section and may have a harder time getting accurate bounds on your graph.

5.3 Unanswered Questions and Action Items

- 1. What determines the maximum achievable purity? the two diffusion coefficients? What is the relationship here
- 2. more thoroughly investigate the competing effects of width
- 3. look at derivatives of concentration profile?
- 4. investigate how using a more accurate description of velocity would effect diffusion
- 5. investigate the assumptions,