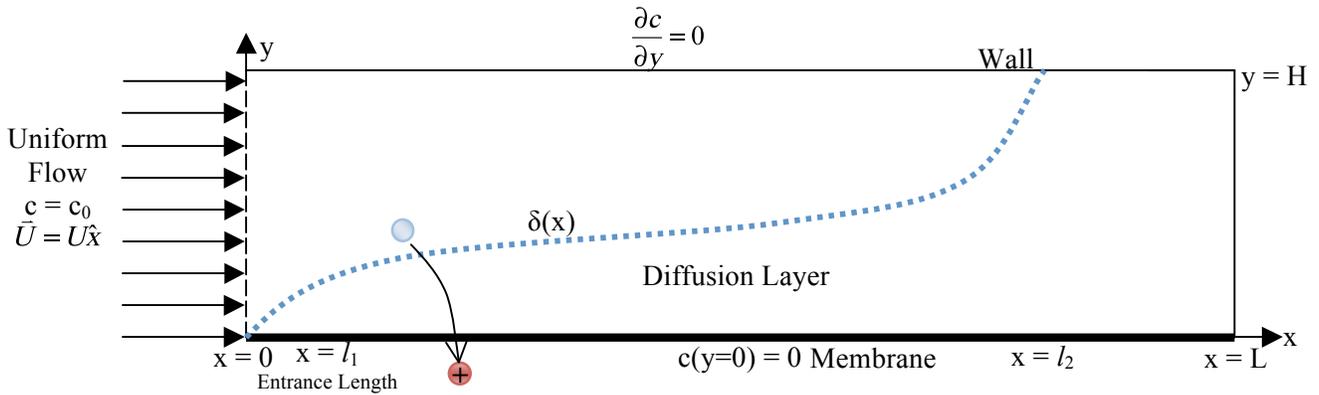


## IV. Transport Phenomena

### Lecture 18: Forced Convection in Fuel Cells II

MIT Student (and MZB)

As discussed in the previous lecture, we are interested in forcing fluid to flow in a fuel cell in order to increase the limiting current, and thus the power output of the device. The model problem considered has a steady uniform flow of fluid carrying the reactant at a constant concentration,  $c_0$ , into a 2-D channel of height  $H$ . In this model we will assume that the fluid velocity profile across the channel is uniform (i.e. plug flow). We are interested in analyzing the transport of the reactant carried into the system by the convective fluid stream to the active membrane located at  $y = 0$ , which has a length of  $L$ .



**Figure 1:** Model problem of forced convection in a fuel cell

From conservation of mass, there is a balance between convection and diffusion terms:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \left[ \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right] \quad [1]$$

Since the flow is steady, the transient term can be neglected. In the region when  $x \gg l_1$ , convection dominates over axial diffusion:

$$u \frac{\partial c}{\partial x} \gg D \frac{\partial^2 c}{\partial x^2}, \text{ when } x \gg l_1 \quad [2]$$

From scaling analysis, we can define  $l_1$  as the point where convection occurs at the same scale as axial diffusion. That is:

$$U \frac{c}{l_1} \sim D \frac{c}{l_1^2} \rightarrow l_1 = \frac{D}{U} \quad [3]$$

Nondimensionalizing the position variables as follows leads us to the Péclet Number,  $Pe$ . Let:

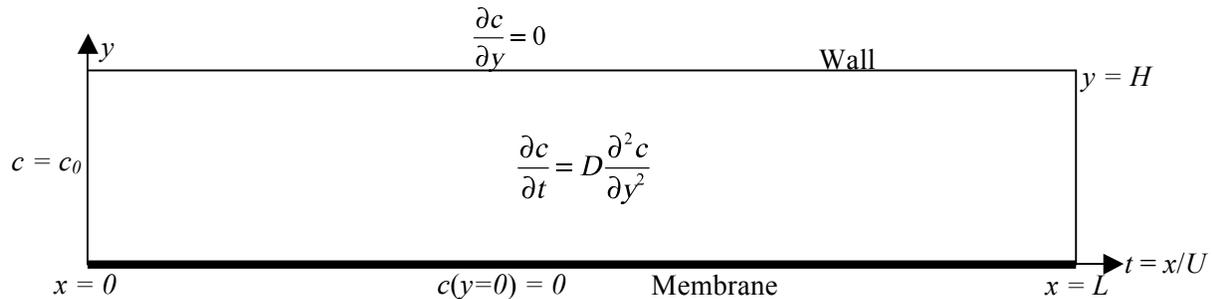
$$\tilde{x} = \frac{x}{H}, \quad \tilde{l}_1 = \frac{l_1}{H} = \frac{D}{UH} = \frac{1}{Pe} \quad [4]$$

In the region where  $x \gg l_1$  or  $\tilde{x} = 1/Pe$ , we can neglect axial diffusion and define a “time” variable  $t = x/U$  along the streamlines to obtain a 1D diffusion equation in terms of  $y$  only. This approach is valid because the fluid flow rate is invariant with location in our model. It is worth restating that the Péclet Number is a dimensionless value that represents the ratio of the rate of convection to the rate of diffusion in the system. We can redefine Equation [1] as:

$$\boxed{\frac{\partial c}{\partial t} = u \frac{\partial c}{\partial x} \cong D \frac{\partial^2 c}{\partial y^2}} \quad [5]$$

and the “initial condition” at the inlet becomes:  $c(x = 0, y) = c(t = 0, y) = c_0$ .

We are now ready to calculate the limiting current  $I_{lim}$  as a function of the fluid velocity,  $U$ , under the assumption that reactions are fast enough everywhere for  $c(t, y = 0) \rightarrow 0$  along the entire membrane when  $I \rightarrow I_{lim}$ . The problem has now become:



**Figure 2:** 1D diffusion model for forced convection in a fuel cell

The limiting current is found by integrating the transverse mass flux along the membrane:

$$I_{lim} = ne \int_0^L D \frac{\partial c}{\partial x}(x, y=0) dx \quad [6]$$

Below we will obtain an exact solution as a *Fourier Series*, but it is more accurate and easier when  $x$  or  $t$  is small to find a boundary-layer similarity solution (as if  $H \rightarrow \infty$ ) in the “entrance region”.

## 1. Entrance Region

Using scaling analysis, the boundary layer thickness,  $\delta(x)$ , can be found:

$$U \frac{c}{x} \sim D \frac{c}{\delta^2} \rightarrow \delta \sim \sqrt{\frac{Dx}{U}} \quad [7]$$

Now we can define  $x = l_2$  to be the axial location where the boundary layer first spans the entire height of the channel, that is  $\delta(l_2) \sim H$  as illustrated in Figure 1. Therefore:

$$l_2 = \frac{UH^2}{D} \quad [8]$$

For  $l_1 \ll x \ll l_2$ , the boundary layer is much thinner than the channel height. Thus, we can set  $H = \infty$ . If we nondimensionalize  $l_2$  and  $\delta$ :

$$\tilde{l}_2 = \frac{l_2}{H} = \frac{UH}{D} = Pe, \quad \tilde{\delta} = \frac{\delta}{H} = \sqrt{\frac{Dx}{UH^2}} = \sqrt{\frac{x}{l_2}} = \sqrt{\frac{\tilde{x}}{Pe}} \quad [9]$$

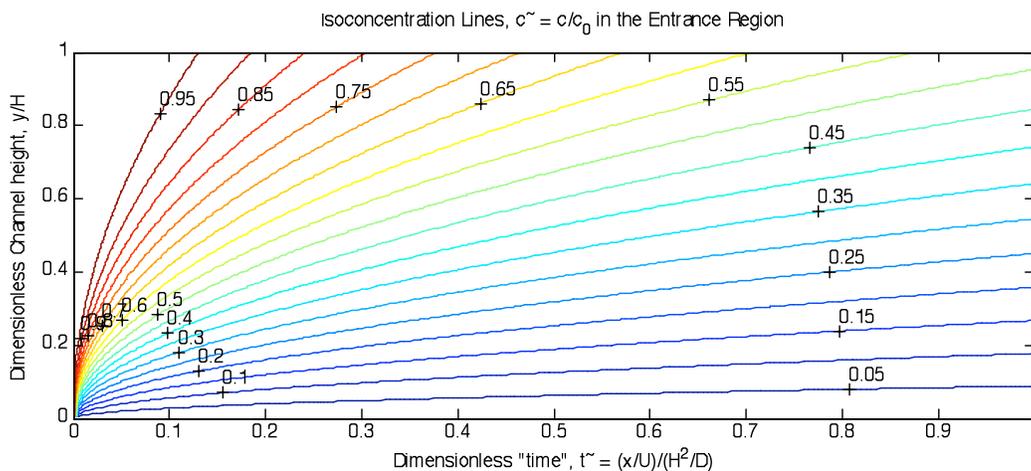
we see that we need  $1/Pe \ll \tilde{x} \ll Pe$  in order to use the boundary layer approximation, which is only valid for small boundary layers, i.e. when  $Pe \gg 1$ .

With  $H = \infty$  (i.e. the boundary layers are so thin compared to the channel height that we can solve using a semi-infinite channel instead of one with finite height), we have a similarity solution to the diffusion equation:

$$c(t, y) \sim c_0 \operatorname{erf}\left(\frac{y}{2\sqrt{Dt}}\right) = c_0 \operatorname{erf}\left(\frac{y}{2\sqrt{Dx/U}}\right) \quad \text{or} \quad \tilde{c}(t, y) = \frac{c}{c_0} \sim \operatorname{erf}\left(\frac{y}{2\delta(x)}\right) \quad [10]$$

Note that here  $y/\delta(x)$  is the “stretched” or “inner” coordinate of the boundary layer and that the error function,  $\operatorname{erf}$ , is defined as:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} ds \quad [11]$$



**Figure 3:** Isoconcentration Lines for Entrance Region

Now that the concentration profile is known as a function of distance along the membrane, we can calculate the flux density,  $F$ , on the membrane:

$$F = D \frac{\partial c}{\partial y}(y=0) = D \frac{2}{\sqrt{\pi}} \frac{c_0}{2\delta(x)} = c_0 \sqrt{\frac{DU}{\pi x}} \quad [12]$$

From above, it is evident that the largest flux occurs near the inlet when  $x \rightarrow 0$ .

Another dimensionless number that is commonly used is the Sherwood Number,  $Sh$ , which represents the ratio of convective to diffusive mass transport. Here it is a dimensionless flux:

$$\tilde{F} = \frac{F}{Dc_0} = \frac{c_0 \sqrt{\frac{DU}{\pi x}}}{\frac{Dc_0}{H}} = \sqrt{\frac{UH^2}{\pi Dx}} = \sqrt{\frac{Pe}{\pi \tilde{x}}} = Sh \quad [13]$$

## 2. Fully Developed Region

For  $x \geq l_2$  or  $\tilde{x} = O(Pe)$ , we can still neglect axial diffusion, however we must solve the full problem for a finite channel height,  $H$ . First, let us define more dimensionless variables:

$$\tilde{y} = \frac{y}{H}, \quad \tilde{t} = \frac{x/U}{H^2/D} = \frac{x}{l_2} = \frac{\tilde{x}}{Pe}, \quad \tilde{c} = \frac{c}{c_0} \quad [14]$$

We can now redefine the diffusion problem as:

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{\partial^2 \tilde{c}}{\partial \tilde{y}^2} \quad [15]$$

with initial condition:  $\tilde{c}(0, \tilde{y}) = 1$ , and boundary conditions:  $\tilde{c}(\tilde{t}, 0) = 0$  and  $\frac{\partial \tilde{c}}{\partial \tilde{t}}(\tilde{t}, 1) = 0$ . This problem can be solved with Fourier Series, or more generally by “Finite Fourier Transform”<sup>1</sup>, as a general series expansion in separable solutions to the PDE:

$$\tilde{c}(\tilde{t}, \tilde{y}) = \sum_{n=0}^{\infty} \theta_n(\tilde{t}) \phi_n(\tilde{y}) \quad [16]$$

where  $\theta_n(\tilde{t})$  is the transform (“FFT”) and  $\phi_n(\tilde{y})$  are the basis functions, determined by the following general procedure. The series expansion is needed since the boundary conditions are inconsistent with a single separable solution.

### 2.1 Step 1 - Determine the Basis Functions

Generally, to solve  $\frac{\partial \tilde{c}}{\partial \tilde{y}} = L_{\tilde{y}} c$  we want the basis functions,  $\phi_n(\tilde{y})$ , to be eigenfunctions of the linear operator  $L_{\tilde{y}}$ :

$$L_{\tilde{y}} \phi_n = -\lambda^2 \phi_n = \phi_n'' \rightarrow \phi_n = A_n \sin(\lambda_n \tilde{y}) + B_n \cos(\lambda_n \tilde{y}) \quad [17]$$

and satisfy the homogeneous boundary conditions:

$$\begin{aligned} \phi_n(\tilde{y} = 0) &= 0 \text{ since } \tilde{c}(\tilde{t}, \tilde{y} = 0) = 0 \\ \phi_n'(\tilde{y} = 1) &= 0 \text{ since } \frac{\partial \tilde{c}}{\partial \tilde{y}}(\tilde{t}, \tilde{y} = 1) = 0 \end{aligned} \quad [18]$$

<sup>1</sup> See W. M. Deen, *Analysis of Transport Phenomena*.

After applying the BC's it is seen that:  $B_n = 0$  and  $\lambda_n = (n+1/2)\pi$ . Therefore, we have the series:

$$\boxed{\phi_n = A_n \sin(\lambda_n \tilde{y})} \quad [19]$$

This method is most useful if this set of functions satisfy the definition of *orthogonality*, which is a generalization of perpendicular vectors to infinite dimensions. Two functions  $\phi_n$  and  $\phi_m$  are said to be orthogonal if:

$$\langle \phi_n, \phi_m \rangle = \int_0^1 \phi_n(\tilde{y}) \phi_m(\tilde{y}) d\tilde{y} = \delta_{m,n} = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases} \quad [20]$$

Furthermore, we choose  $A_n$  so that  $\langle \phi_n, \phi_n \rangle = \int_0^1 |\phi_n|^2 d\tilde{y} = 1$ , which makes the set **orthonormal**.

A crucial property of our linear operator  $L$  (including its boundary conditions) is that it is *self-adjoint*, meaning that  $\langle \phi_1, L\phi_2 \rangle = \langle L\phi_1, \phi_2 \rangle$ , since this implies that the its eigenfunctions are orthogonal<sup>2</sup>

It is then found that:

$$\boxed{\int_0^1 \phi_n(\tilde{y}) \phi_m(\tilde{y}) d\tilde{y} = \int_0^1 (A_n \sin(\lambda_n \tilde{y}))^2 d\tilde{y} = A_n^2 \int_0^1 \sin^2(\lambda_n \tilde{y}) d\tilde{y} = A_n^2 \left(\frac{1}{2}\right) = 1} \quad [21]$$

$$\therefore A_n = \sqrt{2}$$

## 2.2 Step 2 - Transform the PDE into an ODE

Now let's substitute our assumed solution, Equation [16], into the PDE of Equation [15]:

$$\frac{\partial}{\partial \tilde{t}} \left( \sum_{n=0}^{\infty} \theta_n(\tilde{t}) \phi_n(\tilde{y}) \right) = \frac{\partial^2}{\partial \tilde{y}^2} \left( \sum_{n=0}^{\infty} \theta_n(\tilde{t}) \phi_n(\tilde{y}) \right) \quad [22]$$

$$\sum_{n=0}^{\infty} \theta_n'(\tilde{t}) \phi_n(\tilde{y}) = \sum_{n=0}^{\infty} \theta_n(\tilde{t}) \phi_n''(\tilde{y}) = -\sum_{n=0}^{\infty} \lambda_n^2 \theta_n(\tilde{t}) \phi_n(\tilde{y})$$

A property of eigenfunctions is that both sides of the PDE must be equal to  $-\sum_{n=0}^{\infty} \lambda_n^2 \theta_n(\tilde{t}) \phi_n(\tilde{y})$ .

(We are essentially performing separation of variables and setting both sides equal to the same constant, but we can only do it for each term involving a single basis function). Now that the basis functions are orthogonal, the coefficients must be equal:

<sup>2</sup> More generally, all Sturm-Liouville differential operators of the form

$$Lu = \frac{1}{w(x)} \frac{d}{dx} \left( -p(x) \frac{du}{dx} + q(x)u(x) \right) \text{ with homogeneous Robin boundary conditions}$$

$u + a \frac{du}{dx} = 0$  are self adjoint with respect to the inner product,  $\langle \phi_1, \phi_2 \rangle = \int \phi_1(x) \phi_2(x) w(x) dx$ , so

the eigenfunctions of such operators (which come up often in convection-diffusion problems, e.g. Bessel functions in cylindrical coordinates) are automatically orthogonal and convenient for series expansions.

$$\theta'_n(\tilde{t}) = -\lambda_n^2 \theta_n(\tilde{t}) \quad [23]$$

which yields the solution:

$$\theta_n(\tilde{t}) = C_n e^{-\lambda_n^2 \tilde{t}} \text{ and } C_n = \theta_n(\tilde{t} = 0) \quad [24]$$

### 2.3 Step 3 – Evaluate the Constants Using Initial and Boundary Conditions

Because  $\tilde{c}(\tilde{t} = 0, \tilde{y}) = 1$ , we have:

$$1 = \sum_{n=0}^{\infty} \theta_n(\tilde{t} = 0) \phi_n(\tilde{y}) = \sum_{n=0}^{\infty} C_n \phi_n(\tilde{y}) \quad [25]$$

To invert the transform, take the inner product with  $\phi_m$ :

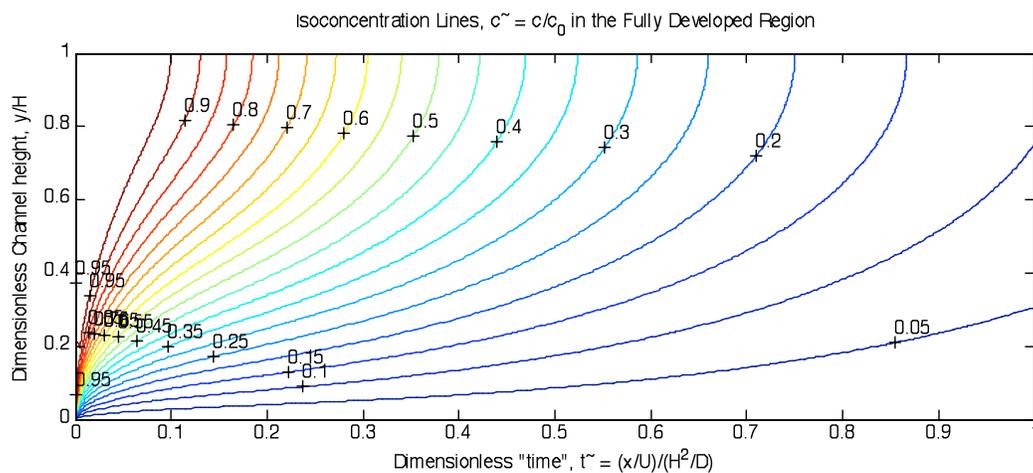
$$\langle 1, \phi_m \rangle = \sum_{n=0}^{\infty} C_n \langle \phi_n, \phi_m \rangle = C_m \quad [26]$$

Using orthonormality:

$$C_m = \int_0^1 \sqrt{2} \sin(\lambda_n \tilde{y}) d\tilde{y} = \sqrt{2} \frac{1 - \cos(\lambda_n)}{\lambda_n} = \sqrt{2} \frac{1 - \cos\left(\pi\left(n + \frac{1}{2}\right)\right)}{\pi\left(n + \frac{1}{2}\right)} = \frac{\sqrt{2}}{\pi\left(n + \frac{1}{2}\right)} \quad [27]$$

Now that the coefficients have been determined, we can put it all together to form the solution:

$$\tilde{c}(\tilde{t}, \tilde{y}) = \sum_{n=0}^{\infty} \theta_n(\tilde{t}) \phi_n(\tilde{y}) = \sum_{n=0}^{\infty} \frac{2}{\pi\left(n + \frac{1}{2}\right)} e^{-\left(n + \frac{1}{2}\right)^2 \pi^2 \tilde{t}} \sin\left(\pi\left(n + \frac{1}{2}\right)\tilde{y}\right) \quad [28]$$



**Figure 4:** Isoconcentration Lines for Fully Developed Flow Region

For  $\tilde{t} \gg 1$  (or  $x \gg l_2$ ) in the fully developed region, the first term in the series dominates:

$$\begin{aligned} \tilde{c}(\tilde{t}, \tilde{y}) &\sim \frac{4}{\pi} c_0 e^{-\frac{\pi^2 \tilde{t}}{4}} \sin\left(\frac{\pi}{2} \tilde{y}\right) \\ \tilde{c}(\tilde{t}, \tilde{y}) &\sim \frac{4}{\pi} c_0 e^{-\frac{\pi^2 x}{4 l_2}} \sin\left(\frac{\pi}{2} \frac{y}{H}\right) \end{aligned} \quad [29]$$

And the flux is:

$$F = D \frac{\partial c}{\partial y}(y=0) \sim \frac{2c_0 D}{H} e^{-\frac{\pi^2 x}{4 l_2}} \quad \text{or} \quad [30]$$

$$Sh = \tilde{F} \sim 2e^{-\frac{\pi^2 \tilde{x}}{4 Pe}} \quad [31]$$

Finally, we can calculate the **limiting current**,  $I_{lim}$ , by integrating the mass flux over the membrane:

$$I_{lim} = ne \int_0^L F(x, y=0) dx, \quad \tilde{I}_{lim} = \frac{I_{lim}}{neL \frac{Dc_0}{H}} dx = \frac{1}{\tilde{L}} \int_0^{\tilde{L}} \tilde{F} d\tilde{x} \quad [31]$$

where  $\tilde{L} = \frac{L}{H} = \text{aspect ratio}$ .

The **fuel utilization**,  $\gamma_{lim}$ , is defined as the ratio of the fuel consumed to the fuel input into the fuel cell:

$$\gamma_{lim} = \frac{\text{fuel consumed}}{\text{fuel input}} = \frac{I_{lim}/ne}{UHc_0} \quad [32]$$

$\tilde{I}_{lim}$  and  $\gamma_{lim}$  are related by:

$$\gamma_{lim} = \frac{\tilde{I}_{lim} LDc_0/H}{UHc_0} = \tilde{I}_{lim} \frac{\tilde{L}}{Pe} = \tilde{I}_{lim} \frac{L}{l_2} \quad [33]$$

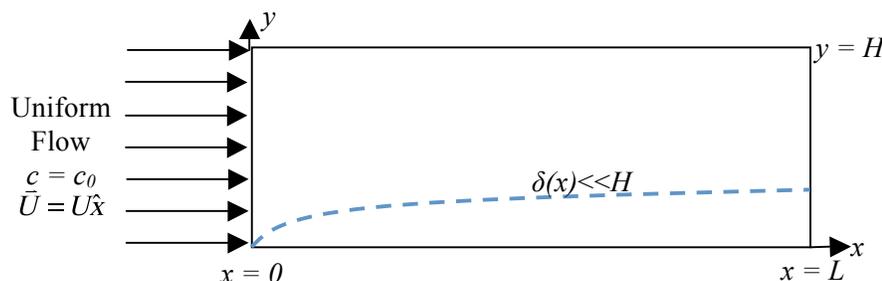
At a given fuel utilization we can boost the limiting current and thus the power,  $P = IV$ , by having *fast flow* ( $Pe \gg 1$ ) and *thick channels*, which allow more fuel into the system.

## 2.4 Flow Regimes

Let's examine the limiting current and fuel utilization in two flow regimes:

### 2.4.1 Fast Flow ( $l_2 \gg L$ )

In this regime the fluid is moving quickly, which means the boundary layer is thin compared to the channel height. This is equivalent to saying that  $l_2$  is located beyond the axial extent of the membrane ( $0 \leq x \leq L$ ).



**Figure 5:** Fast Flow Regime for a Fuel Cell

If  $\delta(x) \ll H$ , then  $DL/U \ll H^2$  and  $(D/UL)(L/H)^2 \ll 1 \rightarrow Pe(H/L)^2 \gg 1$ . From Equation [13]:

$$\tilde{F} = \sqrt{\frac{Pe}{\tilde{x}\pi}} \rightarrow \tilde{I}_{lim} \sim \frac{1}{\tilde{L}} \int_0^{\tilde{L}} \sqrt{\frac{Pe}{\tilde{x}\pi}} d\tilde{x} = 2\sqrt{\frac{Pe}{\tilde{L}\pi}} \quad [34]$$

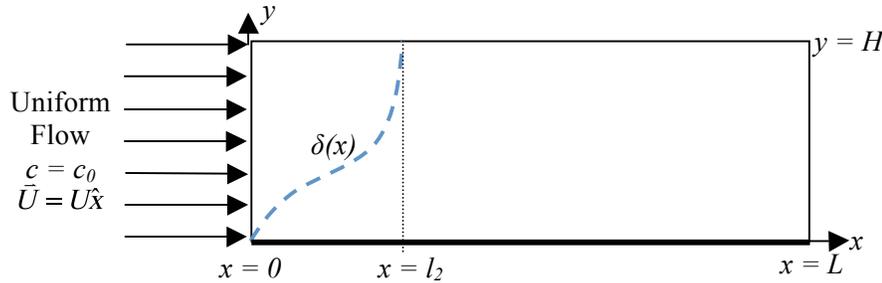
Therefore, the fuel utilization in this regime is:

$$\begin{aligned} \gamma_{lim} &= \tilde{I}_{lim} \frac{\tilde{L}}{Pe} = 2\sqrt{\frac{\tilde{L}}{Pe\pi}} \\ \gamma_{lim} \tilde{I}_{lim} &= 2\sqrt{\frac{\tilde{L}}{Pe\pi}} 2\sqrt{\frac{Pe}{\tilde{L}\pi}} = \frac{4}{\pi} = constant \end{aligned} \quad [35]$$

Because the quantity  $\gamma_{lim} \tilde{I}_{lim}$  is constant in Equation [35], it is obvious that in the fast flow regime there is an inherent tradeoff between power and fuel utilization. That is, although faster flows generate larger power due to an increased  $I_{lim}$ , less of the fuel is able to diffuse to the membrane by the time it reaches an axial position of  $x=L$ .

### 2.4.2 Slow Flow ( $l_2 \ll L$ )

In this regime the diffusion profile is fully developed and the boundary layer has reached the top of the channel for much of the length of the membrane.

**Figure 6:** Slow Flow Regime for a Fuel Cell

Now,

$$\tilde{F} \sim 2e^{\frac{-\pi^2 \tilde{x}}{4 Pe}} \rightarrow \tilde{I}_{lim} \sim \frac{2}{\tilde{L}} \int_0^{\tilde{L}} e^{\frac{-\pi^2 \tilde{x}}{4 Pe}} d\tilde{x} = \frac{8Pe}{\tilde{L}\pi^2} \left( 1 - e^{\frac{-\pi^2 \tilde{L}}{4 Pe}} \right) \quad [36]$$

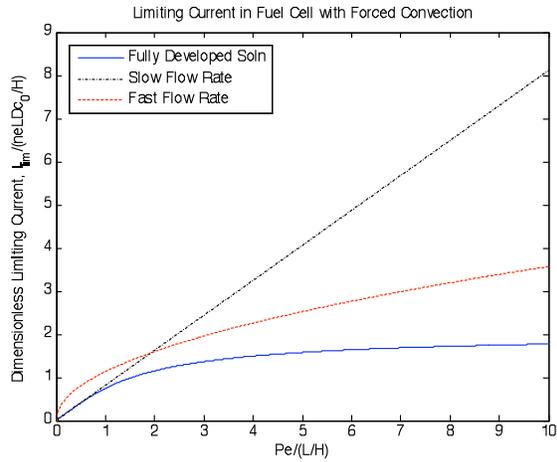
When  $\frac{L}{l_2} = \frac{\tilde{L}}{Pe} \gg 1$ , Equation [34] becomes  $\tilde{I}_{lim} \sim \frac{8Pe}{\tilde{L}\pi^2}$ . The fuel utilization in this case is:

$$\gamma_{lim} = \tilde{I}_{lim} \frac{\tilde{L}}{Pe} \sim \frac{8Pe}{\tilde{L}\pi^2} \frac{\tilde{L}}{Pe} \sim \frac{8}{\pi^2} = constant \quad [37]$$

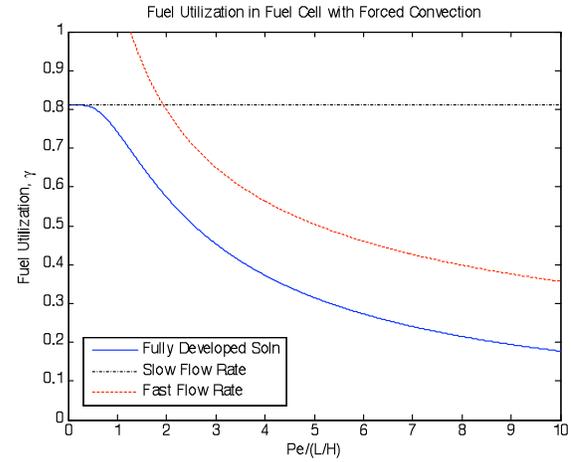
Therefore, for *slow flow* or *long channels*, all of the fuel is consumed, but the power is low.

Note that by keeping only the first term in the Fourier series for the slow flow we found that

$\gamma_{\text{lim}} \rightarrow \frac{8}{\pi^2} < 1$ . To see that  $\gamma_{\text{lim}} \rightarrow 1$  (i.e. all the fuel is utilized), we would need to keep all of the terms in the Fourier series and calculated the exact flux,  $F(x)$ .



**Figure 7:** Limiting Current of Fuel Cell



**Figure 8:** Fuel Utilization of Fuel Cell

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10.626 Electrochemical Energy Systems  
Spring 2014

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