Lecture 7: Introduction to PDEs

Recall that PDEs are differential equations may have one or more dependent variable, and one equation is needed for each, just like ODEs. However, PDEs have more than one independent variable, such as u(x,t) or f(x,y,z,t). Because they allow for both time and space as independent variables, PDEs are required for problems where spatial information is necessary. For example, in lecture one we noted that we would need PDEs to solve a chemical reaction system when transport was slow relative to reaction, a mechanics system when the geometry is too simple for analytic solutions, and a fluid system when inertia of the fluid determined the direction of flow so that the spatial orientation of channels contributed to determining how much fluid flowed into each channel.

This spatial information often adds significant complexity to a system, making it impossible to solve analytically even for simple processes, so PDE models usually require computational solutions. When the complexity of PDE models arises from the complex geometry, the increased complexity does not add uncertainty to the model. The parameters and equations for the geometry can be determined with a high level of certainty from the designed device or a 3D image of the biological structure being modeled. Other properties such as elasticity, diffusion coefficients, and viscosity can often be measured in independent experiments, or may even be known for the materials being modeled, so the parameters in the various physics equations may be well known as well. For these reasons, many PDE models involve very few unknown parameters and thus can be interpreted with a high level of certainty. Because of the need for computational tools for solving PDEs and the relative reliability of PDE models, it is useful for a researcher to learn methods of computational PDE modeling.

In some cases, you are solving a time dependent system, so you have spatial coordinates and time as the independent variables, while in others you are determining equilibrium behavior, so the only independent variables are spatial variables. Numeric solutions to PDEs are obtained by using a mesh to break the space up into small discrete elements, determining the values of the dependent variables at the boundaries, and then interpolating within each of the elements in some manner. Some packages are specialized to solve transport, electrical, or mechanical problems. However, bioengineers have to solve all sorts of different problems, so we use COMSOL in this class because it is a general package that can solve many types of problems separately or in combination, which is why it is now called 'COMSOL multiphysics.' Although we will focus on transport problems, you can use COMSOL to solve other types of problems.

We will not cover analytic time-dependent solutions to PDEs in this class. However, we will learn to calculate steady state solutions and time constants that govern the simulations for simple equations and geometries, in order to verify the simulations.

PDE nomenclature review

<u>Variables</u>: note that your dependent variables can be either scalar (like u(x, y, t) can be the concentration of a chemical), or a vector or even tensor (like v(x, y, t) is the velocity vector of a fluid, which in this case will have two components: $v = (v_x, v_y)$. In this nomenclature review, I am showing two spatial variables, but models can be constructed with 1, 2, or 3 spatial variables, so this is just for illustration.

<u>Partial derivatives</u>: The change in the variable u with respect to time is $\frac{\partial u}{\partial x}(x,t)$, which we sometimes call u_x and the second derivative is $\frac{\partial^2 u}{\partial x^2}(x,t) = u_{xx}$, etc.

<u>Gradient</u>: is the multidirectional spatial derivative, which acts on a scalar variable and returns a vector. It is indicated by the upside-down triangle with the vector notation.

$$\vec{\nabla} u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$$

<u>Divergence</u>: is also like a derivative, but acts on a vector and returns a scalar. It is the sum of derivatives of each element of a vector field with respect to the direction of that element. It is thus like the dot product of a derivative operator and a vector function, and is indicated by an upside down triangle with the dot operation.

$$\nabla \cdot \vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y}$$

<u>Laplacian</u>: is like a second derivative, acting on a scalar and returning a scalar. It is the divergence of the gradient, so is indicated by the square of two upside down triangles.

$$\nabla^2 u = \nabla \cdot \vec{\nabla} u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

<u>Dirichlet Boundaries</u> are prescribed, so the dependent variable at any point on the boundary is defined: (u(boundary) = f(boundary,t)). The prescribed value must have units the same as u, or in concentration.

<u>Neumann boundaries</u> have a prescribed flux normal to the boundary. The normal flux is indicated by $\vec{n} \cdot \vec{J}$, where \vec{n} is the unit vector pointing outward normal to the boundary. The most common Neumann boundary is no flux: $\vec{n} \cdot \vec{J} = 0$. Here, \vec{n} is unitless, and J has units mol/m^2s .

(Generalized) Robin Boundary conditions are a linear combination of prescribed flux and prescribed values. This essentially means that the flux is a linear expression of the value: $\vec{n} \cdot \vec{J} = Au + B$. Since J has units mol/m^2s and u has units mol/m^3 , A must have units m/s, which describes the permeability of a membrane, and B must have units of mol/m^2s , or flux.

For both Neumann and Robin Boundary conditions, we replace the value J in these equations with the equation for flux in the PDE. This will make more sense after some examples.

<u>A note on units</u>: in lecture 2 on building ODE models, we used permeability P in units L/s (or m^3/s), and flux J in units mol/s, because we did not distinguish the geometry of the membranes, so we were aggregating the entire membrane into one item. When we do a PDE model in 3D, we use flux J with units $\frac{mol}{m^2s'}$ and we describe permeability with units m/s. You can see the parallel by realizing that we can integrate the flux or permeability across a membrane over the area of the membrane to convert a PDE to an ODE system. When we model 2D or 1D ODE systems, we use the same units, since we are just assuming an unknown and uniform thickness in the other dimensions. So, our concentration is still in mol/m^3 in 1D, not in mol/m.

Transport equations

Transport equations predict the concentrations of chemicals or particles over time and space. They have the general form of an equation for how the concentration of each species (each variable) changes over time as a result of diffusion, convection, and reaction. This provides a definition for $\frac{\partial \vec{u}}{\partial t}$ in terms of the current value of the vector of species $\vec{u} = (u_1, u_2, ... u_n)$ and any spatial first or second derivatives. To develop the transport equation, we need to calculate the flux J, which is the movement of chemicals to or away from a given spot due to diffusion and convection. Briefly, the transport equation states that the change in concentration of each particle equals the negative of the divergence of the flux plus any change due to chemical reactions.

$$\frac{\partial u}{\partial t} = -(\nabla \cdot J) + rxn$$

<u>Diffusion</u>. Ficks first law states that the flux is proportional to the negative gradient of the concentration. The negative sign indicates that the material moves in the direction of lower concentration.

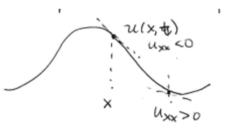
$$\overrightarrow{J_{diff}} = -D\overrightarrow{\nabla}u = -D\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$$

The constant of proportionality, D is the diffusion coefficient. The diffusion coefficient can be measured experimentally by matching macroscale experimental measurements to conditions with a known solution, or by tracking the Brownian dynamics of individual particles, if they can be observed. However, we can calculate or estimate the diffusion coefficient D for a spherical or nearly spherical particle from the Stokes-Einstein equation: $D = \frac{k_B T}{6\pi r \mu'}$, where $k_B T$ is thermal energy ($k_B T = 4.1e - 21 J$ at room temperature), r is the radius of the particle, and μ is the viscosity of the fluid. Note that the diffusion coefficient has units m^2/s .

The diffusion equation says that the concentration changes as the negative of the divergence of the flux. The negative sign here means that the concentration drops if the net flux moves away from rather than towards this point.

$$\frac{\partial u}{\partial t} = -\nabla \cdot J_{diff} = D\nabla^2 u = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

The sense to this can be seen with the 1D interpretation of the Laplacian and the diffusion equation. Consider a curve, u(x,t), that represents the concentration of a chemical at a position x in a 1D channel. Then $\frac{\partial u}{\partial x}$ is the



gradient, indicating how the concentration changes if you move along the channel, and $\frac{\partial^2 u}{\partial x^2}$ is the curvature of this line; if $\frac{\partial^2 u}{\partial x^2} < 0$, the line curves downward, while $\frac{\partial^2 u}{\partial x^2} > 0$ means it curves upward. Because the rate of change in concentration is proportional to the Laplacian and the diffusion coefficient, the concentration drops where curvature is negative, and does so faster for a sharper curvature and faster diffusing species.

<u>Convection</u>. The convection term includes any spatial movement of the species that is not due to diffusion. Chemicals can move along with fluid movement, so fluid velocity must be included in the convection terms. The convection term also includes anything besides concentration gradients that affect the chemical potential. Thus, the convection term also includes movement due to external fields such as electrical or gravitational fields.

We thus let \vec{V} be the velocity of the chemical species due to convection or force fields. Then the flux is $J_{conv} = u\vec{V}$. Thus in a pure convection system, the change in concentration is:

$$\frac{\partial u}{\partial t_{conv}} = -(\nabla \cdot J_{conv}) = -(\nabla \cdot u\vec{V})$$

To illustrate why this is the flux due to convection, we consider a laminar flow parallel plate flow chamber, which we will model in 2D, so $\vec{V} = (V_x, V_y)$. Specifically, there is no fluid movement in the y-direction, so $V_y = 0$, and fluid velocity in the x-direction has a parabolic profile with respect to the height of the element within the chamber: $V_x(x,y) = S\left(y - \frac{y^2}{H}\right)$, where S is the wall shear rate. Velocity in the x-direction is independent of x, so $\vec{V} = (V_x(y), 0)$.

$$\frac{\partial u}{\partial t_{conv}} = -(\nabla \cdot u \vec{V}) = \frac{\partial (u V_x)}{\partial x} + \frac{\partial (u V_y)}{\partial y} = V_x \frac{\partial u}{\partial x}$$

Thus, the concentration changes dependent on the concentration gradient $\frac{\partial u}{\partial x}$ and the speed of fluid movement in the x-direction, as the concentration is a given spot becomes the same is it was a brief time ago at a spot upstream.

Combining diffusion and convection terms gives $J = -D\nabla u + u\vec{V}$, so:

$$\frac{\partial u}{\partial t} = -(\nabla \cdot J) = -(\nabla \cdot (-D\nabla u + u\vec{V})) = D\nabla^2 u - \nabla \cdot u\vec{V}$$

As a final note, if we have convection due to external forces as well as fluid flow, we simply add the two contributions together. The velocity \vec{V} of a particle due to external force depends on the drag coefficient ($\vec{V} = \vec{F}/\gamma$), which in turn depends on the diffusion coefficient ($\gamma = \frac{k_B T}{D}$):

$$\vec{V} = \vec{F}D/k_BT$$

To model convection in a numerical simulation, you may already know the velocity profile, or you may need to solve the Navier-Stokes equations to determine the profile in the case of more complex geometries. To verify the numerical simulation of convection, it is best to eliminate all other terms, so the solution is performed for pure convection; it is often then possible to predict the exact or approximate solution to some set of boundary and initial conditions.

<u>Reaction</u>. When one variable converts to another, we refer to this as a reaction. This could entail an enzymatic reaction, binding between two species, etc. Reactions are also called sources, when a species (variable) is created through reaction, or sinks, when a species reacts (disappears). The reaction terms are thus identical to the ones that would be written for ODE equations. Thus, if chemicals A and B react to form complex C, and all are doing so with convection velocity vector \vec{V} , the complete set of equations has three PDEs:

$$\begin{split} \frac{\partial A}{\partial t} &= D_A \nabla^2 A - \nabla \cdot A \vec{V} - k_{on} A B + k_{off} C \\ \frac{\partial B}{\partial t} &= D_B \nabla^2 B - \nabla \cdot B \vec{V} - k_{on} A B + k_{off} C \\ \frac{\partial C}{\partial t} &= D_C \nabla^2 C - \nabla \cdot C \vec{V} + k_{on} A B - k_{off} C \end{split}$$

This problem will also require boundary conditions and initial conditions for each dependent variable. Note that in this case, all are subjected to the same flow, but each species has a different diffusion constant. If convection was partially due to an external field, then each would also respond to that field differently, and the equations would include species-specific velocities, such as \vec{V}_A .

Verification Tools: Steady State Solutions and Time Constants

We will use two tools:

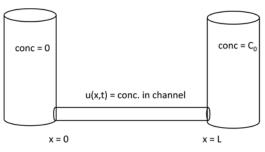
- 1. Most important, we try to identify the steady state solution of a system, which we can compare exactly to the simulation for conditions for which we can obtain it. We find the steady state solution using three steps:
 - a. We *set the time derivatives to zero*. This gives us a second order equation for each variable. We hope we can integrate the solution, or solve in some similar way, but will have two integration constants for each dimension, so this will not provide a complete solution.
 - b. We apply the boundary conditions to narrow down the solution.
 - c. If the system is closed, so that material cannot enter or exit, we will also need to use the initial condition to obtain a unique solution. In this case, we use conservation of mass to set the sum of material in the system at equilibrium to be the same as in the initial conditions.
- 2. We also would like to know the time scale of the simulation. This tells us the expected time frame for reaching steady state, which provides an additional verification and also helps us know how long to run the simulation. We find time constants using three steps.
 - a. Find characteristic times T_i by combining the parameters of the system, including parameters, geometries, etc, in any way that results in something with unit time. For example, if we have a velocity V and a length L, then $T_1 = L/V$ is in units of time and is a possible characteristic time of the system.
 - b. We interpret what each of the time scales mean. That is, each time scale will estimate the time required for some process. For example, $T_1 = L/V$ is the time needed for something moving at velocity V to transit the length L, which determines part of the geometry of the system. When we have more than one time constant, we may be able to provide logic to determine whether the faster or the slower will dominate to overall system time scale, which we will call T_{tot} . That is, we ask whether either process alone could reach steady state, in which case the processes occur in parallel and the faster will dominate $\left(T_{tot} \sim \frac{1}{T_1 + T_2}\right)$, or whether both must occur for steady state, so the processes occur in series, and the slower

- characteristic time slower will dominate $(T_{tot} \sim T_1 + T_2)$. If we can't apply such logic, then we estimate that the system time scale as somewhere in the range of characteristic times: $\min(T_i) < T_{tot} < \sum T_i$.
- c. Use the numeric values of the characteristic times T_i and the overall time scale of the system, T_{tot} , decide how long to run the simulation, and to verify the results. We expect most change to occur in the first one to three T_{tot} , and there is no reason to run the simulation longer than ten times T_{tot} . I usually run the simulation for $3T_{tot}$ at first just to see what is happening, but then will pick the time scale appropriately to show the time dependent response $(3T_{tot}?)$ or to come completely to steady state $(10T_{tot}?)$, depending on the question I am trying to answer.

For many systems we want to model, we cannot calculate an analytic solution for the whole system, which is why we are using numeric methods. However, we may be able to calculate analytic solutions for various components of the system by setting some parameters to zero, by changing boundary conditions, etc. Thus, we hope we can verify that we have built our model correctly with step-wise verification.

Example: Diffusion in a 1D channel.

The channel has length L, and x represents the distance along the channel. The reservoir at x = 0 has no chemical in it, while the reservoir at x = L has concentration C_0 , and the volume of the reservoirs is so large relative to the channel that we consider these concentrations to be fixed. Let u(x,t) represent the concentration of the chemical in the channel at



position x from the left end at time t. We model diffusion in the channel to ask how the concentration in the channel changes over time given several boundary and initial conditions.

<u>Scenario 1: Derichlet boundary conditions</u>. The ends of the channel are open to the reservoirs, so the value is prescribed to remain the same as the reservoir. Also, at time t = 0, there is no chemical in the channel.

Build the model: This example has no convection or reaction, so is the pure diffusion equation: $\frac{\partial u}{\partial t} = D\nabla^2 u$, which in one spatial dimension means:

PDE is:
$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

I.C. are:
$$u(x, 0) = 0$$

B.C. are:
$$u(0,t) = 0$$
 and $u(L,t) = C_0$

- 1. Find the steady state solution, u_{ss}
 - a. Set the time derivative to zero: $0 = \frac{\partial^2 u_{ss}}{\partial x^2}$. Because this system had only one spatial dimension, this is an ODE. We can solve this by integration: $\frac{du_{ss}}{dx} = C_1$, and so $u_{ss}(x) = C_1 x + C_2$. Note that we have two integration constants.

- b. Apply the boundary conditions u(0,t)=0 and $u(L,t)=C_0$ to solve for the two integration constants, C_1,C_2 . Note that boundary conditions might be time dependent, in which case we plug in $t=\infty$. The left boundary gives us $u_{ss}(0)=u(0,\infty)=C_10+C_2=0$, so $C_2=0$. The right boundary gives us $u_{ss}(L)=U(L,\infty)=C_1L=C_0$, so $C_1=C_0/L$. Plugging these in, we obtain $u_{ss}(x)=C_0x/L$.
- c. This is already an exact solution, so we don't need to use the initial conditions. This is expected, since the system is not closed.
- 2. Find the time scale to reach equilibrium.
 - a. The parameters for this system, including boundary and initial conditions, are $D\left(\frac{m^2}{s}\right)$, L(m), $C_0\left(\frac{mol}{m^3}\right)$. The only way to combine these to get units of time is L^2/D . Thus we calculate the characteristic time, $T_1 = L_2/D$
 - b. We interpret this time scale as the time it takes the chemical to diffuse the length of the channel. Since this is the only characteristic time, this is also the time scale of the system: $T_{tot} = T_1$.
 - c. This is the only time scale, so we run the simulation for $\sim 3T_{tot}$ and use a step size of $\sim 0.1T_{tot}$ if we want to plot the time-dependent approach to equilibrium. If we want to plot the distribution at steady state, we might use $10T_{tot}$.

<u>Scenario 2: Neuman no flux boundary condition</u>. Now ask what would happen if we blocked both ends after reaching equilibrium. This is a closed system, where nothing can leave or enter the ends of the tubes, so these are no-flux boundary conditions, which are a type of Neumann boundary. Let's take a moment to understand these boundary conditions, and to translate them into something we can use directly to solve our integration problem.

Recall that the normal flux is indicated by $\vec{n} \cdot \vec{J}$, where \vec{n} is the unit vector pointing outward normal to the boundary. That is, $\vec{n} = -1$ at the left boundary, and $\vec{n} = +1$ at the right boundary. Thus, our no-flux boundary conditions are $-J_x = 0$ at the left boundary and $J_x = 0$ at the right. To translate this, we need to recall what the flux means. In a purely diffusive system, we stated that $\vec{J} = -D\vec{\nabla}u = -D\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$, which in one dimension translates to $J_x = -D\frac{\partial u}{\partial x}$. Thus the boundary conditions are simply $D\frac{\partial u}{\partial x}(0) = 0$, and $D\frac{\partial u}{\partial x}(0) = 0$, or more simply, $D\frac{\partial u}{\partial x}(0) = 0$, and $D\frac{\partial$

Thus, our model is now:

PDE is:
$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

I.C. are: $u(x, 0) = C_0 x/L$
B.C. are $\frac{\partial u}{\partial x}(0) = 0$, and $\frac{\partial u}{\partial x}(L) = 0$

- 1. Find the steady state solution.
 - a. We have the same general solution $u_{ss}(x) = C_1x + C_2$, for the same reason as above.

- b. Apply the boundary conditions, which tell us about the derivative, so we differentiate the solution to get this: $\frac{\partial u_{ss}}{\partial x} = C_1$. Both boundary conditions then give us $C_1 = 0$, so the solution simplifies this time to $u_{ss} = C_2$.
- c. We don't have a unique solution, so we need to use the initial conditions to solve for C_2 using conservation of mass, since the system is closed. To get the total mass, we integrate the initial condition. Instead of using integrals, we realize that the initial condition is a triangle with side C_0 and bottom L, so the area is $C_0L/2$. (The units will be moles/m2, which is correct for our 1D system, because the total mass will depend on the unknown dimensions y and z, or more specifically, the cross-sectional area.) In the steady state solution, the total mass is $Lu_{ss} = C_2L$, so $C_2L = C_0L/2$, and $C_2 = C_0/2$. Thus, the steady state solution is $u_{ss}(x) = C_0/2$.

Thus, at steady state in the closed system, the concentration is constant, and is the average concentration in the initial condition, which makes intuitive sense.

2. We have the same three parameters, so the time scale is the same as in the previous problem.

Scenario 3: generalized Robin conditions. This time we start with zero concentration, but add a membrane with permeability P(m/s) at each end of the channel where it hits the reservior. This is a generalized boundary condition because the flux plus the value is prescribed. Specifically, the flux over the boundary $(\vec{n} \cdot \vec{J})$ equals the permeability P times the difference between the concentration u(x) and the reservoir concentration (either 1 or 0). That is:

$$\vec{n} \cdot \vec{J} = P \cdot (u(x) - 0)$$
 at $x = 0$, or $\vec{n} \cdot \vec{J} = Pu(0)$.
 $\vec{n} \cdot \vec{J} = P \cdot (u(x) - C_0)$ at $x = L$, or $\vec{n} \cdot \vec{J} = Pu(L) - PC_0$

Note that while $0 < u < C_0$, $\vec{n} \cdot \vec{J} = Pu(0) > 0$, so flux is outward on left boundary, and $\vec{n} \cdot \vec{J} = Pu(L) - PC_0 < 0$, so flux is inward on right-hand boundary, which makes sense.

We have the same values for \vec{n} at the two boundaries as in the last example, and we still have $\vec{J} = -D \frac{\partial u}{\partial x'}$ and $\vec{n} = -1$ on the left boundary and $\vec{n} = +1$ on the right boundary, so on the left boundary, $\vec{n} \cdot \vec{J} = D \frac{\partial u}{\partial x}$ and on the right, $\vec{n} \cdot \vec{J} = -D \frac{\partial u}{\partial x}$ We can check the units: \vec{J} , $-D \frac{\partial u}{\partial x}$, Pu, PC_0 all have units of $\frac{mol}{m^2s}$ as required. Also note that both boundary conditions are in the form $\vec{n} \cdot \vec{J} = Au + B$ as required for Robin conditions.

Thus, our model is now:

PDE is:
$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

I.C. are:
$$u(x, 0) = 0$$

B.C. are:
$$D \frac{\partial u(0)}{\partial x} = Pu(0)$$
, $-D \frac{\partial u(L)}{\partial x} = P(u(L) - C_0)$, or $\frac{\partial u(0)}{\partial x} = \frac{P}{D}u(0)$, $\frac{\partial u(L)}{\partial x} = \frac{P}{D}(C_0 - u(L))$

Note that while $0 < u < C_0$, the spatial gradients are positive at both boundaries, so the concentration is always increasing from left to right at both boundaries. This makes sense too.

- 1. Find the steady state solution.
 - a. We have the same general solution $u_{ss}(x) = C_1 x + C_2$, as above.
 - b. Apply the boundary conditions, by substituting $u_{ss}(x) = C_1 x + C_2$ and $\frac{\partial u_{ss}}{\partial x} = C_1$ into $D\frac{\partial u(0)}{\partial x} = Pu(0)$ to get $DC_1 = PC_2$. Similarly, $-D\frac{\partial u(L)}{\partial x} = P(u(L) - C_0)$ becomes $-DC_1 = P(C_1L + C_2 - C_0)$. We solve these two equations simultaneously to find $C_1 = \frac{PC_0}{PL + 2D}$ and $C_2 = \frac{DC_0}{PL + 2D}$ so that the steady state solution is

$$u_{ss}(x) = \frac{PLC_0}{PL + 2D} \cdot \frac{x}{L} + \frac{DC_0}{PL + 2D}$$

 $u_{ss}(x) = \frac{PLC_0}{PL + 2D} \cdot \frac{x}{L} + \frac{DC_0}{PL + 2D}$ This is a line from $\frac{DC_0}{PL + 2D}$ to $C_0 - \frac{DC_0}{PL + 2D}$. If diffusion is fast relative to permeability $(PL \ll D)$, then $\frac{D\dot{C}_0}{PL+2D} \sim \frac{1}{2}$, and this approaches the closed system, while in the opposite situation $(PL \gg D)$, $\frac{DC_0}{PL+2D} \sim 0$, and this approaches the open system.

- c. We don't need to consider initial conditions.
- 2. Find the time scale at which we reach equlibrium.
 - We have the same three parameters, plus P, which is in units of m/s. We still have the characteristic time $T_1 = L^2/D$. However, now we also have $T_2 = L/P$.
 - b. We already noted that $T_1 = L^2/D$ is the time for the chemical to diffuse along the channel. The new characteristic time $T_2 = L/P$ is the time for enough material to enter the channel to fill the entire length of the channel. In order to reach equilibrium, we need the chemical to cross the membrane AND diffuse along the channel. We can't move chemical to the correct position with either of these processes alone. Thus, these processes occur in series, and I expect the system time scale to be $T_{tot} = T_1 + T_2$, which will be dominated by the slower process with the larger characteristic time.