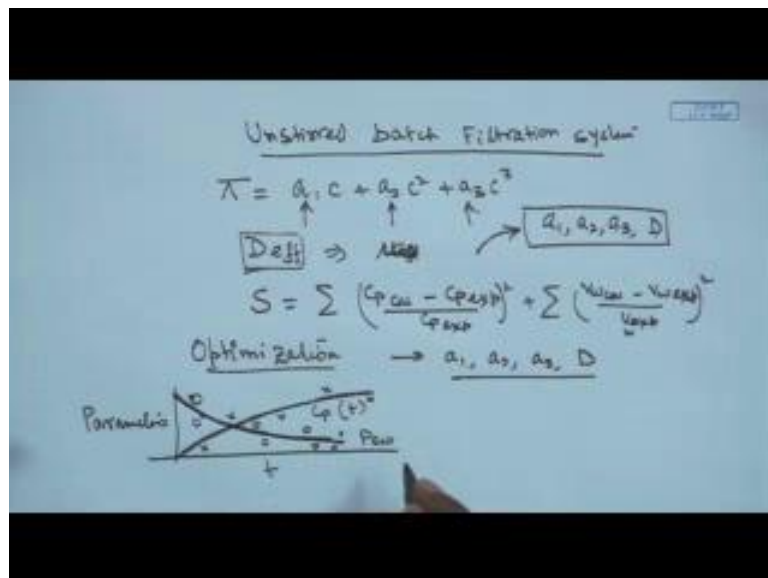


Introduction to Process Modeling in Membrane Separation Process
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Lecture -13
Modeling of Gel Layer Controlling Filtration

Welcome to the session. We will be looking into as we have talked in last class we have finished the as the modeling aspects of osmotic pressure control filtration in a cross flow system.

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Now we will be talking about the importance of unstirred batch system and then will be looking into the modeling of unstirred batch filtration system. Why the unstirred batch system is important that has to be understood first, because if we are talking dealing with a real time with a solution having a solute with unknown properties then it is very easy to solve the system using a predictive mode.

But, suppose we are talking about an industrial effluent or fruit juice or unknown or real life application where there will be not a single component. There are many components present into the system and it is very difficult to identify each and every component;

number 1. Number 2 is that, even if you identify every majority of the components then it will be quite difficult to estimate their concentration. Even if you estimate the concentration now it will be very difficult to estimate their physical property of each and individual material component. For example, their diffusivity, osmotic pressure of the solution things like that.

So therefore, what is generally done; one has taken an effective diffusivity and effective osmotic pressure with a variation of concentration, concentration may be in terms of total solids or total dissolved solids based on the systems. And you will be having an effective osmotic pressure coefficient $a_1 c + a_2 c^2 + a_3 c^3$; a_1, a_2, a_3 may be the you know the effective coefficient osmotic pressure. So, let us write down what are the various parameters those will be appearing $a_1 c + a_2 c^2 + a_3 c^3$ that will be the osmotic pressure of the solution, but we do not know the values of a_1, a_2 and a_3 . And even if you can you have an accurate osmometer. But if you do not know the value of effective diffusivity, effective viscosity and viscosity can be measured of course but the diffusivity value cannot be known.

So, in a typical system you will be having four unknowns; the osmotic coefficients a_1, a_2, a_3 and diffusivity effective diffusivity of the system. So, how this system is then model then what we what is generally done we conduct large number of experiments in the order of 30 40 lot number of experiments and vary the operating conditions and see the permeate flux and permeate concentration and may be in terms of total solids or may be in terms of total dissolve solids.

Once this is done then we go through the model, but we have a profile optimization or the optimization with respect to the experimental values. So we have a guess values, we do a guess values of a_1, a_2, a_3 or D then we go to the model solve the model get the calculated values of permeate flux and permeate concentration for different operating conditions and then we come we compare those values with the experimental data. That means, we minimize the sum $C_p \text{ calculated} - C_p \text{ experimental} / C_p \text{ experimental}$ square of that plus $V_w \text{ calculated} - V_w \text{ experimental} / V_w \text{ experimental}$ square of that; we minimize the sum and optimize the whole system and compare with the experimental data and the module calculated data. Then if this sum is

not less than a tolerance value then again we have to redo a reguess this set of parameters which will be directed by a proper algorithm or minimization algorithm or optimization algorithm.

So, we will be doing an optimization method; optimization for evaluating the system parameters so then a_1 , a_2 , a_3 and D of the system will be predicted will be will be estimated. Once this will be estimated then for an unknown operating condition we can run our model equations in a predictive mode in order to able to predict the system performance.

So, what is the drawback of the system? If you really do a cross flow system then every cross flow system will be under a particular set of operating condition will be giving you one value of permeate concentration and permeate flux, but you will be you require probably huge number of experiments so therefore you have to conduct the cross flow experiment large number of times may be 40 times, 50 times in order to generate you know 40, 50 values of permeate concentration and permeate flux and so you can optimize the four parameter a_1 to a_3 and D effective.

Now that will be then incurring more cost man power energy and material to conduct those experiments. On other hand if you can conduct a batch cell experiment, permeate in a typical batch cell because of the growth of the mass transfer boundary layer one will be getting the permeate flux and permeate concentration profile of that as a function of time. So, we will be getting n number of data. These all be the parameters and usual function of time, the permeate flux will keep on decreasing as a function of time, this will be the permeate flux P_w the non dimensional permeate flux and this how the one dimensional permeate concentration keep on growing as a function of time.

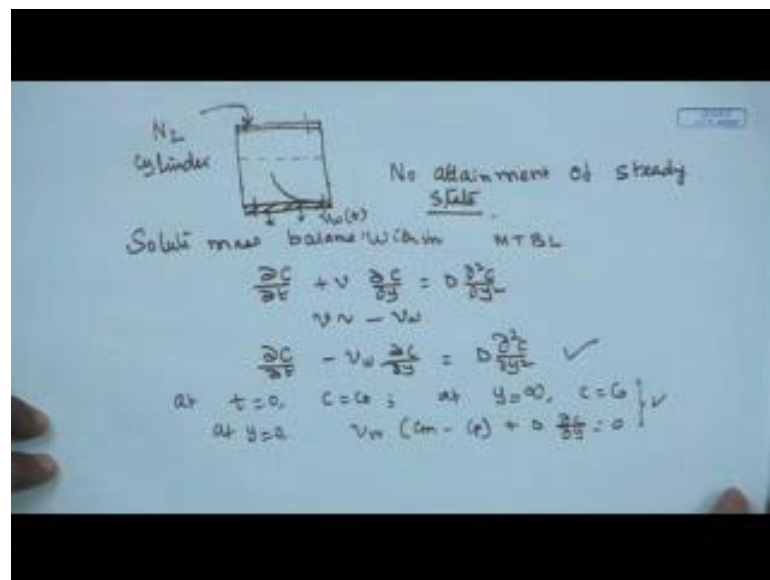
So, what you can do at any fixed time intervals, you can measure the permeate concentration and permeate flux. So you can keep on measuring them, you conduct an experiment for 5 hours; one is single experiment for 5 hours and then you can measure n number of values of permeate concentration pear or permeate concentration permeate flux at different time points. So therefore, if from a single experiment one can generated

data 50, 60 data if you take a run of let us say 2 hours or 3 hours, and if you take data accurately within every 10 minutes or 5 minutes.

So depending on the duration of the experiment one can collect large number of data and those data can be minimized by doing an optimization so that is known as profile optimization. You have the module value of the permeate flux profile and module value of calculated value of permeate concentration profile, you measure the experimental values and plot the experimental values like this. And from a single batch cell experiment one can get a large number of data that is why the modeling of the batch cell all we know filtrations set up is very very important and will be looking into how these modeling can be done.

So, for an actual real system the reger of experiment can be reduced or in order to estimate the parameters quite easily from the bath cell experiment. So, let us look into the modeling of batch cell experiment. What is a batch cell?

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So, it is basically a pressure vessel having three parts; there will be a top flange, there will be a body of shell, there will be a bottom flange and in the bottom flange it will be a circular disc so here will be placing the membrane in the top flange and all these will be

connected to the filtration body of the cell by using nuts and bolts. And then it will pressurize by a nitrogen cylinder, but before that you fill up the cell with let us say 500 ml or 700 ml of solution. So, what will be let us writing down? So, there will be a growth of concentration boundary layer over the membrane surface as we have seen earlier, but in this case there is a difference.

The difference is that in the case of the cross flow filtration the growth of the mass transfer boundary layer will be restricted or arrested by the cross flow of the retentate flow. But in this case so there will be a steady state reached in case of the cross flow filtration, but in the case of unstirred batch cell there is no external agent to curb or arrest growth of the boundary layer. Hence, it will be growing undisturbed and the permeate flux will keep on decreasing as a function of time and permeate concentration will keep on increasing as function of time. So, there will be no attainment of steady state unlike the cross flow filtration cell there is the typical characteristic of a batch cell; no attainment of the steady state.

Thus, what we will do next we will write down the solute mass balance within mass transfer boundary layer. So, if you write it $\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2}$, since mass transfer boundary layer is small we can assume v is equal to minus V_w so that is coming out. And in this case V_w will be function of time, so $\frac{\partial c}{\partial t}$ will be minus $V_w \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2}$. Now, let us set the boundary conditions t is equal to 0, C is equal to C_0 at y is equal to infinity as argued earlier C is equal to C_0 at y is equal to 0. We have all the (Refer Time: 11:17) steady state boundary condition, all the mass fluxes towards membrane surface will be equal to 0; $V_w C_m - C_p + D \frac{\partial c}{\partial y}$ will be equal to 0.

So, this will set up the governing equation and the three boundary conditions. Next what we will do? We make the system non dimensional from very beginning. So, let us do that.

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Handwritten mathematical derivation on a whiteboard:

$$C^* = \frac{C}{C_0}; \quad y^* = \frac{y}{R};$$

$$\frac{\partial C^*}{\partial t} - \frac{V_w}{R} \frac{\partial C^*}{\partial y^*} = \frac{D}{R^2} \frac{\partial^2 C^*}{\partial y^{*2}}$$

$$\Rightarrow \frac{R^2}{D} \frac{\partial C^*}{\partial t} - \frac{V_w R}{D} \frac{\partial C^*}{\partial y^*} = \frac{\partial^2 C^*}{\partial y^{*2}}$$

Parabolic PDE

$$\tau = \frac{t D}{R^2}$$

$$\frac{\partial C^*}{\partial \tau} - P_{ew} \frac{\partial C^*}{\partial y^*} = \frac{\partial^2 C^*}{\partial y^{*2}} \quad P_{ew} = \frac{V_w R}{D}$$

at $\tau = 0, C^* = 1$; at $y^* = 0 \Rightarrow \frac{\partial C^*}{\partial y^*} + P_{ew} C^* R_r = 0$
 at $y^* = \infty, C^* = 1$

So, we define these non dimensional parameters as C star is equal to C by C naught y star is equal to y by R, R is radius of the batch cell. Now let us look into governing equations. This becomes del C star del t minus Vw del C star R del y star and D del square C star divided by R square del y star square. Now multiplied by R square by D so it becomes R square by D del C star del t minus Vw R over D del C star del y star is equal to del square C star del y star square. So, the right hand side is completely non dimensional, the second term in left hand side that is non dimensional, so this is again non dimensional permeate flux this case here.

So, here C star is non dimensional t is dimensional, that means t D by R square has to be non dimensional. That means, we define non dimensional time as t D divided by R square. This becomes del C star del tau minus Pw del C star del y star is equal to del square C star del y star square, so this is the governing equation where Pw is equal to Vw R over D. And now we will be making the boundary to be non dimensional as well. So, at tau is equal to 0 C star is equal to 1 at y star is equal to 0 del C star del y star plus Pw Cm star Rr equal to 0 at y star equals to infinity C star is equal to 1. So, that sets up the governing equation and the boundary condition.

Next again will be taking request to the similarity solution because this is a parabolic partial differential equation and one of the boundary is residing at infinity. So, we can have a similarity solution, so let us have a similarity solution and before that we have to find out what is the similarity parameter; so again will be doing the same order of magnitude by evaluating this concentration profile at edge of the boundary layer.

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$$\frac{\partial C^*}{\partial \tau} = \frac{\partial C^*}{\partial \delta^2}$$

$$\Rightarrow \delta \propto \sqrt{\tau}$$

$$\eta = \frac{y^*}{\delta} + \frac{y^*}{\sqrt{\tau}}$$

$$\frac{\partial C^*}{\partial y^*} = \frac{\partial C^*}{\partial \eta} \frac{\partial \eta}{\partial y^*} = -\frac{1}{\delta} \frac{\partial C^*}{\partial \eta} = -\frac{1}{2} \frac{\partial C^*}{\partial \eta}$$

$$\frac{\partial C^*}{\partial \tau} = \frac{\partial C^*}{\partial \eta} \frac{\partial \eta}{\partial \tau} = \frac{1}{\sqrt{\tau}} \frac{\partial C^*}{\partial \eta}$$

$$\frac{\partial^2 C^*}{\partial y^{*2}} = \frac{\partial}{\partial y^*} \left(\frac{\partial C^*}{\partial y^*} \right) = \frac{\partial}{\partial \eta} \left(\frac{\partial C^*}{\partial \eta} \right) = \frac{\partial^2 C^*}{\partial \eta^2}$$

So, if we really do that $\frac{\partial C^*}{\partial \tau}$ will be $\frac{\partial C^*}{\partial \delta^2}$ and $\frac{\partial C^*}{\partial \tau}$ will be $\frac{\partial C^*}{\partial \delta^2}$ the second term will be gone, so that will be $\frac{\partial C^*}{\partial \delta^2}$ divided by δ^2 . So, δ^2 will be varying as root of τ in this case. Now, we will be getting a similarity parameter; similarity parameter is y^* by δ it will be y^* by root of τ so that will be the similarity parameter will be working with in this particular problem. Next as you have done earlier will be replacing all the partial derivative in the governing equation in terms of the similarity parameter, and let us first find out the similarity the partial derivative of the those will be appearing in the governing equation in terms of the similarity parameter. Once we get those expressions we are going to substitute those expressions in governing equation.

So, $\frac{\partial C^*}{\partial \tau}$ will be nothing but $\frac{\partial C^*}{\partial \eta} \frac{\partial \eta}{\partial \tau}$ and these becomes $-\frac{1}{2} \frac{\partial C^*}{\partial \eta}$ and $\frac{\partial C^*}{\partial y^*}$ will be $\frac{\partial C^*}{\partial \eta} \frac{\partial \eta}{\partial y^*}$ and $\frac{\partial \eta}{\partial y^*}$ is nothing but $\frac{1}{\delta}$

by $2 \frac{d^2 c^*}{d\eta^2}$. Then $\frac{d^2 c^*}{d\eta^2}$ becomes $\frac{d^2 c^*}{d\eta^2}$ and this becomes $\frac{1}{\sqrt{\tau}} \frac{d^2 c^*}{d\eta^2}$ and $\frac{d^2 c^*}{d\eta^2}$ becomes $\frac{1}{\tau} \frac{d^2 c^*}{d\eta^2}$. So now, we are going to substitute these partial derivatives in the governing equation and see what we get.

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The image shows a whiteboard with the following handwritten mathematical work:

$$\frac{d^2 c^*}{d\eta^2} = -\left(\frac{\eta}{2} + \frac{P_{ew}}{\sqrt{\tau}}\right) \frac{dc^*}{d\eta}$$

Use $P_{ew} \propto \frac{1}{\delta^*} \propto \frac{1}{\sqrt{\tau}}$

$$P_{ew}\sqrt{\tau} = A = \text{constant}$$

$$\frac{d^2 c^*}{d\eta^2} = -\left(\frac{\eta}{2} + A\right) \frac{dc^*}{d\eta}$$

at $\eta = 0 \Rightarrow \frac{dc^*}{d\eta} + A c^* R_r = 0$ ✓

at $\eta = \infty, c^* = 1$ ✓

$$\frac{dc^*}{d\eta} = K_1 \exp\left(-\frac{\eta^2}{4} - A\eta\right)$$

$$\Rightarrow c^*(\eta) = K_1 \int \exp\left(-\frac{\eta^2}{4} - A\eta\right) d\eta + K_2$$

So, what we get is that $\frac{d^2 c^*}{d\eta^2}$ is equal to $-\left(\frac{\eta}{2} + A\right) \frac{dc^*}{d\eta}$. And as we have already seen that δ^* is inversely proportional to the $\sqrt{\tau}$, so this will be the P_{ew} right. P_{ew} is inversely proportional to δ^* and δ^* is directly proportional to $\sqrt{\tau}$ therefore $P_{ew}\sqrt{\tau}$ is constant. And this constant let us say this is A .

If that is the case then the ordinary differential equation of second order now becomes $-\left(\frac{\eta}{2} + A\right) \frac{dc^*}{d\eta}$. And now you change the boundary conditions in terms of similarity parameter η $\eta = 0$ $\frac{dc^*}{d\eta} + A c^* R_r = 0$ and at $\eta = \infty$ $c^* = 1$. So, we can will be able solve this equation. So, solution is as we have see earlier $\frac{dc^*}{d\eta}$ is equal to $K_1 \exp\left(-\frac{\eta^2}{4} - A\eta\right)$ and then 1 more integration we will be giving you c^* is function of η $K_1 \int \exp\left(-\frac{\eta^2}{4} - A\eta\right) d\eta + K_2$.

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$K_1 - ARr K_2 = 0$
 $K_1 I_1 + K_2 = 1$

$$I_1 = \int_0^{\infty} R \sqrt{\eta} (-\frac{\partial^2 c}{\partial \eta^2} - A) d\eta \quad (2)$$

$$K_1 = -\frac{ARr}{1-ARr I_1}$$

$$K_2 = C_m^* = \frac{1}{1-ARr I_1} \rightarrow \text{Eq. (2)}$$

Darcy's Law: $P_w(\tau) = B (1 - \frac{\Delta \pi}{\Delta p}) \quad (1)$

Algorithm:

- (i) guess C_m^*
- (ii) P_w from Eq. (1)
- (iii) A can be evaluated from the expression of $P_w \Rightarrow A = \frac{P_w}{\tau}$
- (iv) Evaluate I_1 from Eq. (2)

(v) Evaluate C_m^* from Eq. (3)

(vi) $|C_m^{*_{\text{cal}}} - C_m^*| < \epsilon$

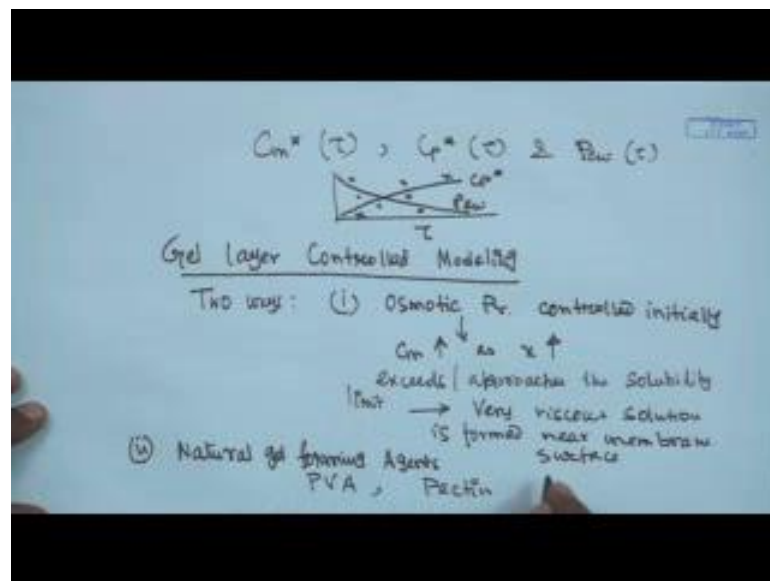
And then using the boundary conditions; this two boundary condition one can evaluate the integration constant K_1 and K_2 as $k_1 + ARr K_2 = 0$ and $K_1 I_1 + K_2 = 1$. Where I_1 is basically the definite interval 0 to infinity $\int_0^{\infty} R \sqrt{\eta} (-\frac{\partial^2 c}{\partial \eta^2} - A) d\eta$ and K_1 becomes $-\frac{ARr}{1-ARr I_1}$ and K_2 is nothing but C_m^* is equals to $\frac{1}{1-ARr I_1}$. And we have the osmotic pressure model so Darcy's law to the porous membrane. P_w as the function of time will be nothing, but $B (1 - \frac{\Delta \pi}{\Delta p})$ you have already seen that $\Delta \pi$ can be expressed as a function of C_m^* .

Now, the model equations complete let us look into the algorithm of calculation. The algorithm calculation is very simple. First at a particular time point τ we do following; one guess C_m^* evaluate P_w from equation 1, once you get P_w from equation 1 then we can get the expression of A , from the expression of A can be evaluated from the expression of P_w . Once that is done then you can evaluate I_1 from equation 2. Once that is done one can evaluate C_m^* from equation 3. So therefore, the equation expression of P_w is nothing but A is equal to $P_w \text{ root over } \tau$.

So, A is equal to $P_w \text{ root over } \tau$ so at that particular τ we put the value of τ we have already evaluated P_w , so P_w multiplied by root by τ will be giving you the value of A .

Substitute A in integral I 1 and evaluate definite integral using (Refer Time: 22:35) rule and get the value of I 1 from the equation 2. And from equation 3 you will be getting the value of C_m star. And check whether this calculated C_m star now C_m star calculated minus C_m star guess the less than epsilon naught, if they are less than epsilon go for next time step t plus Δt if not then you have to re guess the value of C_m star and repeat the iterative calculation.

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So, in the process what you will be getting is that, if the process will be ultimately getting C_m star as a function of time C_p star as a function of time and P_w as a function of time, so ultimately you will be getting P_w as the function of time and C_p star as a function of time. And you will be having measured value of P_w at different time points and measured value of C_p star defined time points then you can do the optimizations and can estimate the system parameters. So, that is how the batch cell filtration can be done.

So, this completes our whole formulation for the modeling or content for the modeling of of the osmotic pressure filtration both in the cross flow cell and the batch cell. We have first started with one dimensional model we went ahead with the two dimensional model and by observing several short comings of the one dimensional model and we have seen that one dimensional model will really will give the under prediction of permeate flux.

And therefore, we went ahead with two dimensional model completely solve the two dimensional model for the cross flow filtration system as well as the batch system filtration system. Also we have iterated that discussed about the importance of batch cell; why it is so important for evaluating the system parameter or the process parameters whenever you will be working with a real industrial field or real fruit juice sample.

Next type of modeling will be looking into the Gel Layer Control Modeling. Under two circumstances a gel are very highly viscous solution is prepared on the membrane, this is formed on the membrane surface there are two ways; first way is that the filtration may be osmotic pressure control initially and then during the osmotic pressure control filtration membrane surface solute concentration of the membrane surface keep on increasing as you move down stream of the channel. And therefore at a particular location it may happen that it exceeds the solubility limit; exceeds or approaches the solubility limit.

In that case once it does that then a very viscous solution is formed near membrane surface and if the solubility limit is exceeded at that particular temperature there may precipitation of the solute as solute phase. Or there may be another way is a natural gel forming agency. There is some natural gel forming agents, for example polyvinyl alcohol, pectin etcetera. These solutes they form a gel over the membrane surface from the very beginning.

So, you do not need to give time of them for formation of gel, they already form they from the very beginning of the filtration the form a solute gel type of they form a highly viscous solution, so highly viscous layer near the membrane surface. And this gel keeps on going in time with time of operation or duration of operation in the y direction over the membrane surface. There are two typical ways how the gel formed.

In the next class we will be looking into the various types of gel polarization model. And how the various parameters will be estimated in a typical gel polarization model which will basically be taking few from the classical filtration theory and combine it and will bring those you know concepts in the gel layer formation, and then will looking into how the gel layer modeling can be done.

Thank you very much.