

Mathematical Modelling and Stimulation of Chemical Engineering Process

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Lecture 24

Modelling transport phenomena problems - part 4

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Mathematical modelling and simulation of chemical engineering process
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Lecture 24 : Modelling transport phenomena problems – part 4

CONCEPTS COVERED

- ❖ Solvent induced heavy oil recovery
- ❖ Moving boundary problem



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Hello everyone, in this lecture, we are going to see a very important transport process related to oil recovery. So, all of you are aware of that oil is an essential resource, which provides us energy, so extraction of oils is a very engineering challenge as well as a very important or a vital platform for technological inputs.

So, oil recovery techniques have been studied for the past almost like 30 to 40 or 50 years almost. And there are several techniques which have been incorporated during this process, one of the, a popular way that has been evolved in the last decade or so is that using solvents a solvent induced oil recovery methods.

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Solvent assisted gravity drainage (SAGD)

Assumption

1. Shape of the reservoir—cylindrical
2. Solvent penetrates uniformly from all sides of the reservoir
3. Oil + solvent mixture flows down vertically, due to gravity.
4. Ignore temp. effects. (5) No chemical rxn

oil reservoir (heavy oil)

Low viscosity Solvent

CO₂, propane, methane, etc.

Drainage (oil + solvent mixture)

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6. Density of the solvent mixture is constant.
7. Diffusion along the axial direction is small compared to convection.
8. Gravity drainage starts after the solvent is introduced.

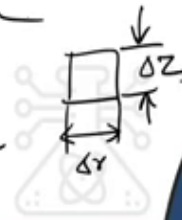
Solvent mass balance.

$$\frac{\partial}{\partial t} (\rho \phi \omega \Delta V) = \left[N_r A_r |_r - N_r A_r |_{r+\Delta r} \right] + \left[N_z A_z |_z - N_z A_z |_{z+\Delta z} \right]$$

ω : solvent mass fraction

ρ : density of the oil-solvent mixture

ϕ : porosity of the reservoir



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Now, what essentially this means that you are going to have an, let us say you have a oil reservoir or a porous domain which contains oil. Let us assume that domain or that reservoir to be something like a cylindrical space, which contains the oil. Now, to this an oil I mean the major challenge in oil recovery is that since it is highly viscous, I mean crude oils are generally highly viscous, there is a huge pressure drop and huge pressure requirements which makes the problem or the recovery or the extraction quite challenging as well as technologically complex.

So, one of the methods that was devised is that if you can induce some low viscosity solvent into this heavy oil and essentially, they should be compatible or miscible and, in the process, the overall viscosity can be reduced resulting in easy recovery. One of the ways that this is done is there is something known as a solvent assisted gravity drainage and this is a technique that is very popularly used in oil sands in Canada these days, this is known as the SAGD process.

So, what is done in this process that in this oil reservoir, so this is an oil reservoir which contains this the heavy oil and into this you try to inject some low viscosity solvent which is of course to a greater extent miscible or compatible to the oil or to the hydrocarbon and in this process the oil viscosity reduces and it tries to drain out from this reservoir which can essentially be then collected, so this is the drainage from this reservoir, so this is the oil solvent mixture.

So, later on since this low viscosity solvent are generally, so what are the popular choice of this low viscosity solvent, this could be carbon dioxide, this could be propane, it could be also methane, steam could also be a possibility but it is not very much preferred because for steam you need to have a high temperature process, but and generally these are the popular choices CO₂, propane in a methane and this also utilizes a lot of extent to the CO₂ which is that again a greenhouse gas.

So, the important thing to realize is this after this oil solvent mixture is drained out or is recovered very easily, these low viscosity solvents which is generally have high volatility or even by the change of pressure you can generally have a phase extraction and these heavy oils have very high boiling points, so they can be easily separated out. So, this is a popular method which is known as the solvent assisted gravity drainage.

Now, in this case if you are trying to mathematically model the system and understand what is the flow rate, what is the concentration of the oil and all those things, I mean that this is what this modelling is supposed to tell you, it is very important to frame the appropriate mathematical equations.

So, in this case we assume that the shape of the reservoir, so let us write down the assumption. So, here we make an assumption that a shape of the reservoir is cylindrical, shape of the reservoir is cylindrical. We also assume that this solvent penetrates almost uniformly from all sides of the reservoir. Third assumption we say that the oil solvent mixture this flows down vertically and due to gravity, no additional pressurization is required for this gravity drainage problem.

So, as such this oil zone, let us say the oil zone in this, let me mark it with a different colour, the oil zone in this reservoir actually decreases in its volume or in its vertical height with time as time progresses the oil reservoir depletes, so it is sort of a moving boundary problem, because the size of the oil domain itself reduces. So, when the zone of the, so this is the active zone at let us say at certain time T after the process has started.

So, this tells you that this shape of the cylinder or essentially the size of the cylindrical domain actually changes or evolves with time. There are some more important assumptions we ignore let us say any temperature effects in the problem, then we have no chemical reaction.

Another important assumption is that the density of the solvent mixture is constant. So, you may argue that even let us say if I am trying to inject CO₂ into the system, so as to change its viscosity how come the density is unaffected. So, dense amount density viscosity and diffusivity generally viscosity is the strongest function of concentration or mass fraction followed by diffusivity followed by density.

So, generally with little amount of this gas or whatever this low viscosity solvent added to this heavy oil will not change its density significantly, you can think of an analogous situation is that when you try to inject or will try to bubble air into water does it change the density of the air bubble mixture? it is not, if the density of the bubble I mean if the gas fraction or the air fraction in the water is not significantly high the density is not so much affected.

So, in this process at least for this simplified scenario we consider that the density is unchanged even with the addition of the solvent or the low viscosity solvent. And as another thing we also want to mention here that diffusion in the axial direction, diffusion along the Z direction or the axial direction is small compared to convection. So please note that along the axial direction there is flow due to the gravitational effects. So, there is a strong convection.

So, diffusion in the axial direction is not significantly high or comparable with respect to convection. So, in this problem this is the R direction, so let us say that this boundary is r is equal to capital R and let us also try to write down that this is z is equal to 0 and this is z is equal to let us say capital Z naught or height of the reservoir or the initial height of the reservoir.

So, along the Z direction it is insignificant and we also make another condition that the process or the gravity drainage starts after the solvent, this low viscosity solvent is introduced, so this by this we inevitably assume that there is no leakage and this gravity drainage does not happen without the solvent even if there is to some extent practically, there is some drainage in the system, but that is very much small amount which can be ignored.

So, with all these assumptions, let us try to write down now the solvent balance to the, of the problem. So, if you do a solvent mass balance, we get so this is the accumulation term, so here I am trying to I mean w is the solvent, so let me write w is the solvent mass fraction, ρ is the density of the oil solvent mixture, ϕ is the porosity of the reservoir, which because these rocks or these reserved domains are porous in nature.

So, this is the accumulation term that I have written on the left-hand side, then we have the flux in across the radial direction as well as the axial direction. So, the difference of the fluxes both along the axial direction and radial direction, so this is the radial direction and then also I write the axial direction, so this is the axial direction. So, you can just like thinking about a small elemental section having a radius of delta r and vertical radius or segment of delta Z. So, this is what in the cylindrical section we are trying to write.

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$N_r = -D \rho \phi \frac{\partial \omega}{\partial r}$ along the r-direction.
 $N_z = -\omega \rho V_z$ (no diffusion) in the z-direction.
 $V_z = -\frac{k_0}{\mu(\omega)} \rho g$ (Darcy flow).
 Darcy law $\rightarrow V \propto -\nabla P \Rightarrow V = -\frac{k}{\mu} \nabla P$
 $\Delta V = 2\pi r \Delta r \Delta z$
 $A_r = 2\pi r \Delta z$
 $A_z = 2\pi r \Delta r$
 $\therefore \frac{\partial \omega}{\partial t} = \frac{D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \omega}{\partial r} \right) - \frac{1}{\phi} \frac{\partial}{\partial z} (\omega V_z)$

So, now let us look into the fluxes, so this N_r is the flux along the radial direction and we can write that to be $D \rho \phi$, $d\omega$ by dr from the Fick's law, so this is along the r direction, so in the r direction please note there is no convection to the problem and for the Z direction you have minus ρV_z , because there is no diffusion or diffusion is insignificant in the Z direction. So, it is only convective flux.

Now, how do we write V_z ? So, this V_z is can be written down from the Darcy's law. I hope all of you are aware of what do you mean by Darcy's law. So, Darcy's law helps you to describe the velocity profile in a porous domain and it is generally proportional to the negative of the pressure gradient in the porous domain. So, in this case, so the constant of the equality generally gives you the idea of the permeability of the porous medium K is the permeability of the porous medium.

So, in this case the pressure difference is the gravitational head or the hydrostatic head, so we can write this as $K_0 \rho g$, so K_0 is the permeability of the medium of the porous domain, ρg this is the hydrostatic pressure drop, so K sorry I should write this properly, so it is K , a K is the permeability divided by I mean sorry let me write it properly minus so permeability of the porous medium divided by the viscosity of the mixture which is a function of concentration of the solvent, times ρg . So, this the pressure gradient due to the gravitational effect.

So, this is like Darcy type flow we are having in the porous domain, these elemental sections ΔV is of the small unity of the small cross-sectional element is $2\pi r \Delta r \Delta z$, the projected cross sectional area along the r direction is $2\pi r \Delta z$ and A_z is $2\pi r \Delta r$, I hope all of you understand this the flux along the r direction. So, what is the elemental cross section area and the flux, I mean the A_z is the projected surface area which the flux penetrates in the Z direction that is $2\pi r \Delta r$.

So, with introduction of all these balances it is now we can write down in the limits of Δr tending to 0 and ΔZ tending to 0 we get $\frac{dw}{dt}$ is equal to $\frac{\partial}{\partial r} \left(\frac{D}{r} \frac{\partial w}{\partial r} \right) - \frac{1}{\Phi} \frac{\partial}{\partial z} (v w z)$ and of course $v w z$, $v w z$ is related as $K_0 \rho g$ by μw and μw , so the viscosity is a function of the concentration and we know that w is also changing with time.

So, you can have some relation on how the viscosity is related to the function of the concentration, there are there are several such viscosity relationships which can tell you that how does it depend or how does it vary with the concentration of the solvent, for a mixture these relations are quite well defined.

Now, please realize that to solve this problem, we need boundary conditions and boundary conditions are dependent on the condition that the domain size is changing in this problem. So, we need to have a fair idea on how the vertical height that is what we have assumed that there is no radial shrinkage, but vertically it is going down, so how the vertical height changes with time and to find out that we need to make another balance.

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Oil-solvent mass balance


rate of oil-solvent mass into the system (rate of change of volume) = rate of oil-solvent mass out of the system (production).

$$\Rightarrow \rho \frac{\partial}{\partial t} (\phi \Delta V) = -\rho V_o(r) 2\pi r dr$$

\uparrow $2\pi r dr \Delta z$ $\rightarrow v_{z=0} = \frac{-\rho g k_o}{\mu[\omega(r,0)]}$

$$\Rightarrow \frac{dz}{dt} = -\frac{V_o(r)}{\phi}$$

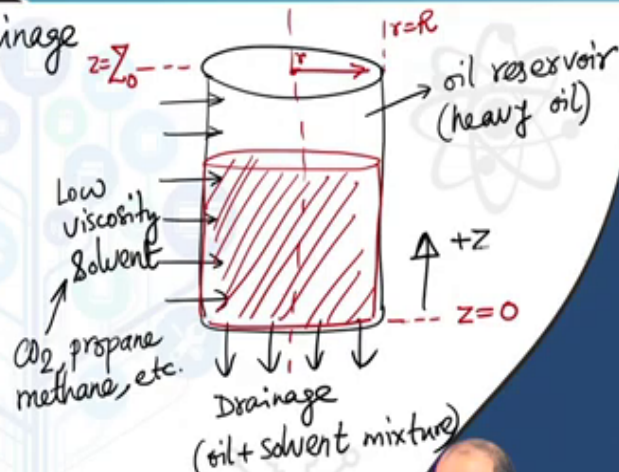
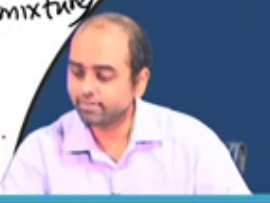
$Z(r,t)$



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So, this is the if I try to make an oil solvent mass balance, I can write that the I mean the idea is that the rate of oil solvent mass into the system is equal to the rate of oil solvent mass out of the system and this is nothing but equal to the production rate, this is nothing but the production rate and this part rate of oil solvent mass into the system is something also can be equated to the rate of change of volume of the oil zone.

So, these can be equated as $\frac{d}{dt} \int \Phi \delta V$ rate of change of the volume and the production rate is since the production rate is out of the system, so I write this on the hand side as I mean the velocity is in the downward Z direction and Z is in the upward direction. So, if you go back to the picture, you will see that the positive X Direction is along this direction, positive X and the velocity is coming out in the minus Z direction, so I can write I have to write this as minus rho and that is $V_0 r^2 \pi r dr$.

So, since this delta V is again dependent on small fraction of delta r and this V_0 is a function of r, how this V_0 is a function of r? Because, what is this V_0 by the way? So, V_0 is nothing but V at z is equal to 0, so V at z is equal to 0 is minus rho g k 0 mu and this value of the mu is at w, I mean since w is a function of both r and z, so this value of the w at different r locations will be different.

So, accordingly the viscosity at will also have a radial variation as well as of course axial or Z directional variation. So, w is a function of r and z and t, so if I am trying to compute the velocity at or the convection at the z is equal to 0 or the drainage rate which is nothing but V, then I have to consider the viscosity effects along the r direction and this is true for I mean different r locations.

So, in this case, I can find out that delta V is not in this case is $2 \pi r dr Z$, so that is the differ, this volume of this segment across a small elemental section of delta r. So, from here I can write out dZ/dt where capital Z is a function of time is equal to minus $V_0 r$ by Phi, so of course the this will have I mean Z at different locations will be different because V_0 is different.

So, at different r locations the shape will not even though I have drawn in the first figure that it will be like uniformly this the height will be uniform at different r locations that may not be the case from this relation.

So, this capital Z this tells you that capital Z, capital Z which is the height of this oil zone is a function of r and t, so it may not have uniformly I mean across the cross section the zone may not deplete uniformly, it depends on how much is the viscosity variation across the cross section. So, this will help you to get an understand that what is my current Z location and based on that the boundary conditions should be satisfied at that Z location.

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IC $w(r, z, t=0) = 0$
 $Z(r=0) = Z_0$

BC. $w = w_i$ @ $r = R$. (solvent injection conc.)
 $\frac{\partial w}{\partial r} = 0$ @ $r = 0$ (symmetry condition)
 $w = w_i$ @ $z = Z(r, t)$ [Top surface].

Heavy oil production: R

$$\frac{dm}{dt} = \rho \int_0^R 2\pi r V_0(r, t) dr$$



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$N_r = -D \rho \phi \frac{\partial w}{\partial r}$ along the r -direction.
 $N_z = -w \rho V_z$ (no diffusion) in the z -direction.
 $V_z = -\frac{k_0}{\mu(w)} \rho g$ (Darcy flow).
 Darcy law $\rightarrow V \propto -\nabla p \Rightarrow V = -\frac{k}{\mu} \nabla p$ $-\frac{k_0 \rho g}{\mu(w)}$

$\Delta V = 2\pi r \Delta r \Delta z$
 $A_r = 2\pi r \Delta z$ $A_z = 2\pi r \Delta r$
 $\therefore \frac{\partial w}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(D \frac{\partial w}{\partial r} \right) - \frac{1}{\phi} \frac{\partial}{\partial z} (w V_z)$



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$$\Rightarrow \rho \frac{\partial}{\partial t} (\phi \Delta V) = -\rho V_o(r) 2\pi r dr$$


\uparrow $2\pi r dr Z$

$$v_{z=0} = \frac{-\rho g k_o}{\mu[\omega(r,0)]}$$



$$\frac{dZ}{dt} = -\frac{V_o(r)}{\phi}$$

$Z(r,t) \rightarrow$ height of oil zone



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So, let us talk about the initial and the boundary condition, so the initial condition is w at I mean initially t is equal to 0, let us say it has a fraction I mean initially there is no solvent in the system, so we can easily consider that to be 0 and this the z initially at r is equal to 0, sorry this capital Z the height of the layer is capital Z naught initially boundary conditions. So, w is equal to w_i at r is equal to capital R , and dw/dr is equal to 0 at r is equal to so this is the solvent entry point, solvent injection wall or the solvent injection concentration or the fraction and this is the symmetry condition.

And since the problem is one dimensional, I mean first order in the Z direction, so we need only one boundary condition in Z . So, I am defining w_i as z is equal to 0 or it is better to consider that on the boundary condition capital Z sorry capital Z so this is small z is equal to capital Z , which is a function of r and time, so this is the top surface.

So, the net heavy oil production rate this is something which is a very important parameter for industrial significance. So, let us write that as dm/dt , so mass of the oil produced per unit time is $2\pi r \rho$ and then we do a radial averaging of this quantity. So, let us write it properly, so that is $\rho 2\pi r V_o(r, t)$, so this is the heavy oil production which is the value of the velocity or the convective rate convection rate at the bottom wall of this case and which is something we already know that it is dependent on the viscosity values and for that we have to solve out the concentration profile of this problem.

So, w is the solvent mass fraction this equation tells you that how w is a function of r , z and t and in this equation it relates you how the boundary or the axial dimension actually shrinks as with time leading to depletion of the oil zone and this height of the, so this is nothing but the height of the oil zone, height of oil zone is a function of the radial distance and time, so it may happen that radially it may not shrink at the same rate and there is radial diffusion of the solvent. So, the viscosity variation radially is not uniform and that may lead to difference in the height of the oil zone across the cross section with time.

So, the likely scenario or the more realistic scenario can look something like let me see how I can draw, so if this is the initial oil zone shape, so with time it is likely to evolve something like this, so this is the Z , so there will be more drainage from the side walls because the at the side while the solvent concentration is more and leading to the low values of viscosity at the side wall.

So, the convection rate at the side or along the r direction I mean at the near the wall of this system will be will be more compared to the centre, so you will have more oil that is going out from the sides in the central region will have less oil, I mean will have less oil production rate I mean that is the likely scenario in this case.

So, this equation actually helps you to relate that how Z capital Z which is the height of the oil zone changes with radial dimension and time and the heavy oil production rate is there I mean is an important parameter or important metric to compute that from this reservoir process or a simulation how much oil you can expect to get with respect to time.

So, I hope all of you got the essential message in this problem, which is a very engineering relevant problem in oil recoveries considering a moving boundary problem. So, in this case we do not consider the radial shrinkage as this will make the problem slightly more complicated, but there is something for you to think over and try it yourself that having a shrinkage both in the radial and the vertical direction how you can formulate the problem. I hope all of you liked this lecture and found it useful. Thank you.