

Multiphase Microfluidics
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Lecture - 16
Taylor Flow: Mass Transfer

Hello. So, in this lecture we are going to continue our discussion of Mass Transfer in the Taylor flow regime. In the previous lecture we discussed about the basics of mass transfer some non-dimensional numbers and the general features of mass transfer in the Taylor flow regime. In this lecture we will try to use that knowledge to develop some of the models or we will discuss some of the models that have been developed in the literature in last 1520 years.

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Mass Transfer Model: Gas-Liquid



- > van Baten and Krishna (2004) model: *Validated with CFD modelling*
 - > Considered the contributions from caps and the liquid film

$$k_L a = k_{L, \text{cap}} a_{\text{cap}} + k_{L, \text{film}} a_{\text{film}} \quad \text{(Rising Taylor bubble in a Capillary)}$$

- > Cap contribution using Penetration model:
 - Caps are considered to be hemispherical
 - The liquid molecule remains in contact with bubble caps along a distance which is half of bubble cap circumference

$$= \frac{\pi d_b}{2} \approx \frac{\pi d}{2}$$

contact time $\theta = \frac{\pi d}{2 U_B}$

$$a_{\text{cap}} = \frac{\pi d_b^2}{\frac{\pi}{4} d^2 L_{oc}} = \frac{4}{L_{oc}} (d = d_b)$$

$$k_{L, \text{cap}} = \sqrt{\frac{D}{\pi \theta}} = \alpha \sqrt{\frac{D}{\frac{\pi}{\pi d} (2 U_B)}} = \frac{2\sqrt{2}}{\pi} \sqrt{\frac{D U_B}{d}}$$

diffusivity

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So, we will start with the mass transfer for gas liquid transfer. So, for a Taylor bubble as we have discussed several times that one can look at a unit cell, and the bubble the best approximation in terms of simplified geometry for the bubble can be the spherical caps and the cylindrical middle portion.

So, for gas liquid mass transfer Van Baten and Krishna from university of Amsterdam, they considered the mass transfer from gas bubble to the liquid phase and considered the

contributions, from the bubble caps at the front and rear and the cylindrical middle the film region separately.

So, one can write $K_L a$ which is the overall gas liquid mass transfer coefficient into the interfacial area, that is equal to $K_L \text{ cap}$ into a cap plus $K_L \text{ film}$ into a film. So, first we will consider the contribution from the caps and for simplification for geometrical simplification caps are considered to be hemispherical. The diameter of channel is d and let us say the diameter of the bubble is d_b .

Now, in our picture of the derivation that they did for was for a rising Taylor bubble in a capillary and then it was validated with extends the CFD models bar CFD modelling. So, in the near the Taylor bubble as we have discussed that there is recirculation in the liquid zone.

So, the a if the flow is in this direction, then the a liquid particle comes on this side and move and then it goes. So, the recirculation or a liquid particle and it recirculates inside the liquid slug it comes into the contact with the this much length of the bubble.

Similarly, on the other side so, let us just consider the other side of the bubble on, the other side when the so, this the bubble is moving in this direction. So, then the liquid comes in contact with the bubble interface the cap and then again.

So, in a liquid molecule the entire distance or the it remains in contact with bubble caps along a distance, which is half of bubble cap or the circumference.

So, the average distance travelled is equal to πd_b the entire circumference this side and this side and the half of this will be $\pi d_b / 2$ and we can assume this that d_b is equal to d_c neglecting the small film thickness. So, for thin film thickness one can have this d_b is equal to the channel diameter, which is by this. So, you write is $\pi d / 2$.

Now, contact time in this case will be so, when we have the length is $\pi d_b / 2$ the contact time θ will be length over distance. So, $\pi d / 2$ and the velocity of the bubble let us say is U_B . So, the contact time will be $\pi d / 2$ divided by U_B .

Now, from the penetration theory $K_L \text{ cap}$ is equal to $D / \pi \theta$ into 2. So, that will be equal to $2 \sqrt{D} / \pi \pi d / 2 U_B$ this will be equal to $2 \sqrt{2} / \pi \sqrt{D} U_B$ divided by $D / 2 \sqrt{2} / \pi d U_B$ by d . So, remember this D is

molecular diffusivity or mass diffusivity and small diameter a small is small d channel diameter U B is velocity of the bubble and if it is not known a priori we can take this almost to be equal to U D B.

Now, the other thing we need to know is a cap. So, a cap is equal to this will be divided by the cross sectional is divided by the volume of the unit cell. So, that will be pi by 4 d square LUC and the surface area of 2 hemispheres together put together will be one hemisphere. So, that will be pi d b squared ok. So, that will eventually be 4 by LUC with the assumption that d is almost equal to d b. So, we have calculated the mass transfer coefficient and the interfacial area density for the bubble caps ok.

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Mass Transfer Model: Gas-Liquid

Gas holdup or void fraction
 $\epsilon_g = \frac{L_B}{LUC}$

→ Film contribution using Penetration model: contact time $\theta_{film} = \frac{L_B}{U_B} = \frac{\epsilon_g LUC}{U_B}$

$$k_{L, film} = 2 \sqrt{\frac{D}{\pi \theta_{film}}} = 2 \sqrt{\frac{D U_B}{\pi \epsilon_g LUC}}$$

$$a_{film} = \frac{\pi d_b L_B}{\frac{\pi}{4} d^2 LUC} = \frac{4 d_b L_B}{d(LUC)} = \frac{4 \epsilon_g}{d} \quad (d_b = d)$$

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Now, coming to the contribution from the film region so, for the film region again one can define KL film is equal to 2 square root of D over pi theta in contact with the film. Now theta film can be defined as the length of the bubble theta is contact time. So, contact time for the film can be defined as the length of the bubble the film region divided by UB.

And if we define epsilon G, which is void fraction or gas hold up, it can be defined roughly equal to L B over LUC which will hold good for long bubbles and long unit cell because the volume of the spherical caps can be neglected in that case. So, we can have LB replaced by epsilon G LUC divided by U v. So, that gives us K L film is equal to 2 square root of D over pi and theta film epsilon G L U C and U B.

Now, we can write the total contribution. So, that is $K_L a$ is equal to $K_L \text{ cap}$ plus $K_L \text{ cap}$. So, before we do that we also need to find a film. So, it is like a film now a film is equal to the volume of the unit cell which will be $\pi d^2 L U C$ and the surface area will be $\pi d l$ for this cylindrical region.

So, that will be $\pi d b$ into $L B \pi$ and π will cancel out and that will be $d b L B 4$ divided by $d L U C$ and for the case and $d b$ is approximately same as d we can write this as $4 \epsilon G L B$ by $L U C$ can be written as ϵG . So, $4 \epsilon G$ and this is D square. So, $4 \epsilon G$ over D . So, that is the K_L and al film.

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Mass Transfer Model: Gas-Liquid

➤ Film contribution using Penetration model:

$$k_L a = \frac{2\sqrt{2}}{\pi} \sqrt{\frac{D U_B}{d}} \frac{4}{L_{uc}} + 2 \sqrt{\frac{D U_B}{\epsilon_G L_{uc} \pi}} \frac{4 \epsilon_G}{d}$$

Rectangular channels:-

- δ_f is not uniform.
- Bubble caps are not hemispherical.

$$k_L a \approx \sqrt{\frac{D U_B}{d}} \left[\frac{8\sqrt{2}}{\pi} \frac{1}{d} \frac{1}{L_{uc}} + \frac{8\sqrt{\epsilon_G}}{\pi L_{uc}} \frac{1}{d} \right]$$

↑ Channel diameter
 ↑ Unit cell length

Good agreement with CFD simulations

- found that mass transfer is dominant in the film region.

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So, we can now write the total contribution which is $K_L a$ is equal to $K_L \text{ cap}$ into a L cap. So, $K_L \text{ cap}$ is let us go back to $2 \sqrt{2}$ over π into $\sqrt{D U B}$ over d a cap is 4 over $L U C$ plus the contribution from the film is $2 \text{ square root } D U B$ divided by $\epsilon G L U C$ into $4 \epsilon G$ over d . So, let us just check $2 \sqrt{d U B}$ by $\pi \epsilon G L U C$. So, we have $\epsilon G L U C \pi$ then to $4 \epsilon G$ over D .

So, we can see from here that in both the cases $K_L a$ is proportional to $\sqrt{D U B}$. So, the overall mass transfer coefficient it is proportional to the square root of diffusivity and it is proportional to the square root of the velocity of the bubble. The constants we have here inside is $8 \sqrt{2}$ over π into 1 over \sqrt{d} , 1 over $L U C$ plus 2 , then that will again the $8 \sqrt{\epsilon G}$ divided by $\sqrt{\pi}$. So, that is 4 into $8 \epsilon G$ dub already out. So, you will have $\sqrt{\pi L U C}$ into 1 over d .

So, this is basically function of channel diameter and unit cell length. So, that suggests that the mass transfer coefficient will be higher for larger channel diameter and it will be also higher film when the units cell length is shorter will also depend on the volume fraction.

Now when they compared this model with the CFD simulations for mass transfer they had good agreement with CFD simulations and also found, that mass transfer is dominant in the film region.

Now, when it comes to the rectangular channels; because in micro-fluidics; people not only use circular capillaries, but more and more rectangular or square capillaries. So, in the rectangular channels film thickness is not a constant delta F is not uniform everywhere and bubble caps are not necessarily hemispherical.

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Mass Transfer Model: Gas-Liquid

➤ Film contribution using Penetration model:

- Cap mass transfer can be neglected.
- Considered only film contribution

$$k_L a = C_1 \frac{D U_B}{\sqrt{\epsilon_G L_{vc}}} \frac{l}{d} = C_1 \frac{D U_G}{\sqrt{L_{vc}}} \frac{l}{d}$$

$\frac{U_B}{\epsilon_G} = U_G$
known while performing experiments

$C_1 = 4.5 \frac{\beta}{\sqrt{\pi}}$

$$\sqrt{\frac{U_G + U_L}{L_B}} > 3 \text{ OR } Fo < 0.1$$

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So, in their work they further considered a simplified model, where they consider that cap mass transfer can be neglected and then considered the film contribution only. So, K L a in this case will be proportional to a constant C 1. So, on the constants they were brought together under C 1 and then that is equal to D U B by epsilon G L U C 1 over d and U B by epsilon G it can be written as the superficial velocity of gas.

So, this is replaced by a quantity which is known, while performing experiments it is easier to use in the models of C 1 square root of D U G over L U C into 1 over d. And

what they found is that C_1 from their experiments the comparison with the experiments in circular as well as rectangular capillaries that C_1 is 1 about 4.5 the value from the model from the earlier model it was about 8 divided by root pi which is very close to this value.

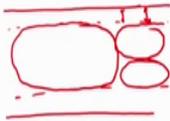
They suggested that applicability of this model was good during their experiments and given a criteria that this will be good when U_G over U_L divided by $L B$ square root of it is greater than 3 or the contact time is less than 0.1 or the Fourier number is less than 0.1.

Now, while using this model 1 need to take into account the fact that is the length of the bubbles and slugs are very long then in that case the film might get saturated and there will be no mass transfer to the film. So, in this case the film will remain in inactive player during the mass transfer so, one need to use this model with a caution; looking at the length of the bubbles and slugs that are generated for a particular configuration.

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Mass Transfer Model: Liquid-Solid

- Higher mass transfer coefficients than liquid only flow
- Liquid-solid mass transfer depends on:
 - Intensity of vortices
 - Thickness of liquid film on the channel wall
 - Surface area provided between liquid and solid phases
- Which translate into
 - Two-phase velocity $U_{TP} = U_G + U_L$
 - Channel dimension (d)
 - Slug length (L_s)
 - Diffusivity (D)



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So, now what we have looked at is mass transfer for gas liquid interface looking at the contributions from the bubble cap and contributions from the film region and we said that in the limit of short contact times it is the mass transfer through the interface in the film region, which is dominant and we gave the relationships for the 2 cases based on penetration theory.

Now, the other region which we need to consider is mass transfer in the liquid solid where the liquid in the slug as well as liquid in the film region may interact with the wall. So, this will depend on the basically on the flow behaviour in the liquid slug. So, as we know that the flow in the liquid slug has internal circulation. So, which has vortices? So, it will depend on the intensity of these vortices and then we have this picture of or this configuration of Taylor bubble that on a thin film the bubbles and slug move. So, it will also depend on this thickness of the liquid film on the wall and the of course, the surface area between the liquid and solid phases.

So, in the parameters that we study this will translate to the 2 phase velocity or U T P, which is some of the superficial velocities of gas and liquid the dimension of the channel d length of the slug and diffusivity D ok.

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Mass Transfer Model: Liquid-Solid

- Two steps:
 - Mass transfer from the vortex to the film
 - Mass transfer from film to the wall
 - Analogy with the developing single phase flow

$$Nu_{sh} = f(Gz)$$

$$Gz = \frac{L}{d Re_{sc}} \left(\frac{v}{D} \right)$$

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So, one can develop a correlation based on the mass transfer considered the 2 region, where in the liquid slug region there is internal recirculations in the liquid slug and the film region and put them put the 2 resistances in series. So, while the mass transfer from the vortex to the film can be considered using the stagnant film model what is what we need to concentrate on or what is to be looked upon is mass transfer from the film to wall.

So, as we have seen in heat transfer during the heat transfer in Taylor flow regime that there is an analogy for the flow in the liquid slug with the single phase developing flow

in a channel. So, same will come into play here and we know that in such case the Nusselt number or Sherwood number for mass transfer this is a function of Graetz number where the Graetz number is a function of l over $d Re Sc$ Sc is Schmidt number ratio of mass diffusivity a momentum diffusivity by mass diffusivity and also number as usual D is the channel length.

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Mass Transfer Model: Liquid-Solid

➤ Kreutzer et al. (2003): For liquid slug

$$Sh = \sqrt{\alpha^2 + \frac{\beta}{Gz}}$$

$$\alpha = 40 \left(1 + 0.28 \left(\frac{L_{slug}}{d} \right)^{-4/3} \right)$$

$$\beta = \left(90 + 104 \left(\frac{L_{slug}}{d} \right)^{-4/3} \right)$$

➤ $Gz =$ Graetz number

➤ For long slugs (and large value of Gz)

$Sh \sim 40$

$Sh = \sqrt{\alpha^2} = \alpha = 40$

$Gz = \frac{L}{d Re Sc}$

$Sh = \frac{dC}{\delta_{channel} \min C_{in}}$

$Sh_{sp} = 3.63$

Entire unit cell (50% void fraction) ≈ 20 $\delta = R$

IIT, Guwahati $\delta = 2R$ $\delta = R$

So, there have been several correlations for defining for modelling the behaviour in the liquid solid region some of them 2 of notable of them, we present here one is by Kreutzer he gave that the Sherwood number is a function of Graetz number where the Graetz number is defined as l over $d Re Sc$ as we seen in the previous slide.

Now, it also have 2 parameters alpha and beta and this alpha this alpha and beta they are weak functions of the non-dimensional slug length. So, we can see that the Sherwood number and in this the l is the length of the channel so, if the slugs are long. So, this can be l slug or l channel depending on what one is considering. So, if the slug is long then this term will go to 0 and what we will have is as such is equal to root of alpha square and where alpha because this term will again be very small compared to one. So, we will have Sh is equal to alpha which is 40.

So, the single phase for the same boundary condition the Sherwood number for single phase flow is 3.63. And so, one can see the one order of magnitude difference the for

this developing flow in the liquid slug the Sherwood number is about 10 times this is for the only liquid slug.

So, if we consider for the entire unit cell with 50 percent void fractions, then also this number will be about 20. So, which is about 5 times the Sherwood number in single phase liquid; single phase liquid flow.

So, this is again further high than the single phase liquid flow. So, a region for this has been suggested by Kreutzer that in the liquid slugs what happens that there is a recirculation and the Sherwood number is basically a non-dimensional gradient at the wall. So, that will depend on the concentration difference divided by a length scale from the channel wall to the minimum concentration.

So, this is channel wall to minimum concentration in case of single phase flow the minimum concentration will be at the centre and so, this δ will be radius of the channel. Whereas, in this case the minimum concentration region will be located at the centre of this vortex and if you remember from the hydrodynamics that we discussed one can calculate the, this distance this is about r over $\sqrt{2}$. So, if you put that will be about point 7 r and this is point 3 r . So, the distance of the minimum concentration for this δ is about point 3 r .

So, this distance has decreased for the Taylor flow plus the another factor that contributes here is that in the single phase flow the liquid at the centre it moves forward in it has a high velocity whereas, in the Taylor flow the liquid at the centre is also brought towards the wall. So, the residence time of all the fluid elements in these slugs are equal whereas, the residence time in this case is there is quite significant distribution of the residence time in single phase flow ok.

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Mass Transfer Model: Liquid-Solid

➤ Van Baten and Krishna (2005)

➤ For wall-slug region

$$Sh = \frac{2.4 + 1.5 \frac{d}{L_s}}{\left(\frac{L_{tube}(1-\epsilon_G)}{d^2 U_B} \right)^{0.45}}$$

Void fraction

➤ For the channel

$$Sh = 0.5 \left(\frac{\epsilon_G}{Gz} \right)^{0.15} Gz^{-0.48}$$
$$Gz = \frac{(1-\epsilon_G) L_{uc}}{d Re Sc}$$

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So, another correlation that has been given by Van Baten and Krishna and both of these correlations are one by Kreutzer and by Krishna they have been developed with extensive validation with CFD modelling. So, Van Baten Krishna they have given 2 correlations one for the wall slug region and one for the entire channel. So, this gives the Sherwood number 2.4 plus 1.5 d over L S and in this case divided by 1 tube 1 minus epsilon G. So, where epsilon G is void fraction d over d square U B and for the channel this is Sherwood number 0.5 epsilon G over G z where the Graetz number in this case is slightly modified.

So, they have considered a Graetz number one minus epsilon G L channel or you can consider L U C divided by d Reynolds number and Schmidt number. So, the difference in this is in terms of and they have multiplied the Graetz number with 1 minus epsilon G. So, considering effectively the length of the slug and they had quite a good agreement with the CFD results and some of the experimental results.

So, these are the correlations for mass transfer and the liquid solid wall. So, another interesting a region, where one would need to have models is for see liquid liquid mass transfer, but to the best of my knowledge there is no not very well developed model especially from the fundamental principles there are several models, which based on the fitting to the experimental data or from the dimensional analysis. So, we are not going to discuss that and I request you to look at the literature for those things. In this lecture

what we have essentially looked at 2 models for the one for the gas liquid mass transfer for Taylor bubble at the interface where we have considered the contributions from the cap and contributions from the film region.

Now, if the bubbles are long and the contact times are large then the film might get saturated and it may become inactive; however, when the contact time is sought it has been observed and the model has been developed for such case that the mass transfer from the film region is the dominant one it will depend on the length of the bubble and the length of the slug. So, a picture one can imagine that when the bubble is in contact with the film the film that gets saturated with the gas and when the slug comes by this mixing happens between the film and the slug.

Now, the other model that we have looked at is mass transfer between the liquid and solid wall. So, one can have a series model there that there are two different regions one is mass transfer from the re-circulating slug to the film in contact with the wall and other is mass transfer from wall film between the film and the wall.

So, for the mass transfer between the film and wall one can use a stagnant film model, where $K_L B$ will be equal to $capitla D$ over δ the film thickness and for the slug region there are 2 models that have been proposed by Kreutzer and Professor Krishna Raj group and both these model are based on the developing a mass transfer or in single phase flow regime with some modifications to those correlations. So, that is all for this lecture.

Thank you.