Chemical Process Intensification
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Module7: Process Intensification by Monolithic Reactor
Lecture 7.4: Hydrodynamics, Transport of Monolithic Reactor

So welcome to massive open online course on Chemical Process Intensification. So we were discussing something about the process intensification by monolithic reactor as a module 7 and under this module 7, we will discuss something more about this monolithic reactor. In this lecture, we will discuss some hydrodynamics, transport processes of monolithic reactor. In this lecture we will cover these different aspects of hydrodynamics. You know that how the liquid will be distributed throughout the monolithic structure and what will be the hold-up of the phases, how the friction or pressure drop is taking part in the chemical engineering process based on this monolithic structure.

And also, what are the mass transfer characteristics of any chemical engineering process will be that carried out through this monolithic reactor?

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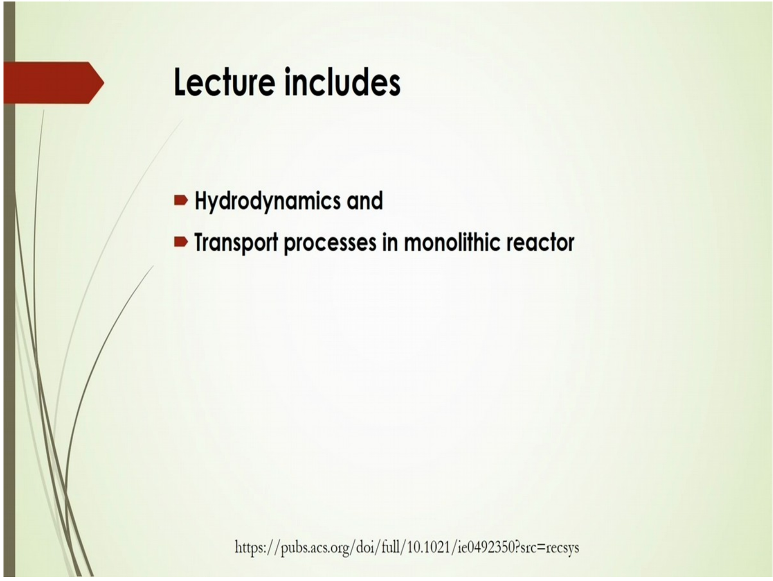

Lecture includes

- Hydrodynamics and
- Transport processes in monolithic reactor

https://pubs.acs.org/doi/full/10.1021/ie0492350?src=recsys

So we will be discussing about that mass transfer characteristics also in this lecture.

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Recap

Monolithic structure support for catalyst

Catalytic reactor

A monolith structure is sometimes referred to as a "honeycomb structure"

Now before going to that, we have to recall again that what is that monolithic structure, what is that? So from the concept of structure, architectural structure of that ancient age, the concept is converted to the present chemical engineering process by developing different structures of that monolithic structure to actually utilise this for the chemical engineering process as it for the process intensification in that particular chemical engineering processes. So based on that structure we are getting different types of structure of monolithic like honeycomb structure, even you can say that some other that Square-based, oval shaped structure, micro-channel based structure, different structure. Already we have discussed the how that different type of structure of monolithic reactor are being actually procured and what are the different methods that we have discussed in the previous lectures.

And also, we have discussed more about that what will be the actually application of that monolithic structure for that particular chemical engineering process based on the process intensification on this particular type of that structured reactor.

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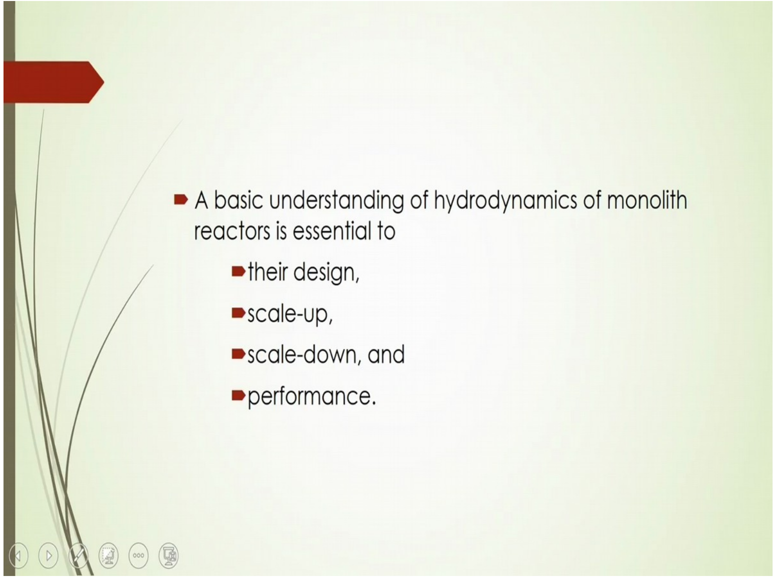

- A basic understanding of hydrodynamics of monolith reactors is essential to
  - their design,
  - scale-up,
  - scale-down, and
  - performance.

Now whenever you are going to perform any chemical engineering process for the process intensification in this particular type of monolithic structured reactor, you have to know something about the hydrodynamic characteristics, what would be the flow behaviour, how liquid will be distributed, what would be the pressure drop, how mixing is happening inside the reactor. For this particular shape of this reactor that you have to know, because this basic understanding of those hydrodynamics of monolithic reactors is essential because of for the design of their particular reactor and it is a scaled-down and also performance of the reactor.

So those things are of course important before going to install that particular monolithic reactor in a particular process in industry.

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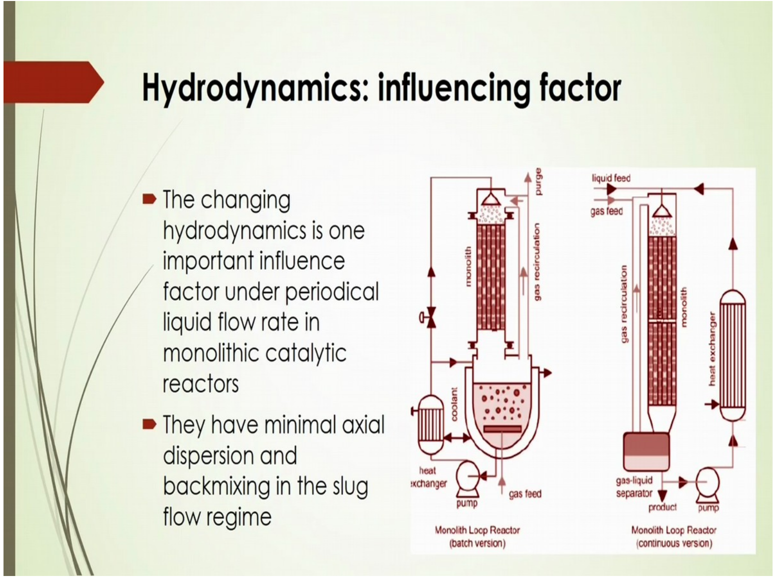

Hydrodynamics: influencing factor

- The changing hydrodynamics is one important influence factor under periodical liquid flow rate in monolithic catalytic reactors
- They have minimal axial dispersion and backmixing in the slug flow regime

And in that case, what are the different factors that affects on that particular hydrodynamics, like that the changing of hydrodynamics based on that geometry, shape of that monolithic structure, even operating variables, even some geometric variables. Like there it is the square shaped micro-channel or ball shaped micro-channel or you can say that rectangular shaped micro-channel or other various types, that depends on that geometry how you are giving this shape of that monolithic reactor and those factors actually will affect the hydrodynamic characteristics in the reactor.

So we can say that the changing of this hydrodynamic is one of the important influencing factor under periodical liquid flow rate in the monolithic catalytic reactors and they have minimal axial dispersion and backmixing in the slug flow regimes that particularly for the micro-channel based structure of this monolithic reactor, that is called honeycomb structure of that monolithic reactor. In that case, micro-channel based that procurement is being done for that special type of this monolithic reactor.

There actually the efficiency of this reactor is being calculated based on that mixing characteristics of the fluid and that mixing characteristics of the fluid depends on the flow pattern of this fluid through that channel based reactor. So in that case, the slug flow regime is one of the important flow characteristic there because for the micro-channel based reactor only this type of slug flow regimes can be obtained where you can, that get that minimum backmixing of the fluid phase in this particular slug flow regime.

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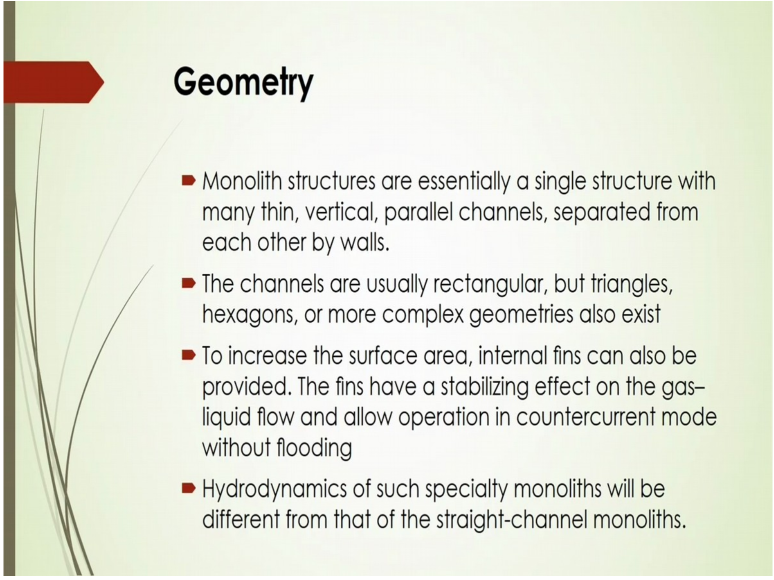

Geometry

- Monolith structures are essentially a single structure with many thin, vertical, parallel channels, separated from each other by walls.
- The channels are usually rectangular, but triangles, hexagons, or more complex geometries also exist
- To increase the surface area, internal fins can also be provided. The fins have a stabilizing effect on the gas–liquid flow and allow operation in countercurrent mode without flooding
- Hydrodynamics of such specialty monoliths will be different from that of the straight-channel monoliths.

And the monolithic structures also essentially are single structure with many thin, vertical, even parallel channels separated from each other by the walls. And in that case, the channels are usually rectangular but sometimes, it may be triangular shaped, sometimes it will be hexagonal and sometimes it will be some other complex, different geometries. There based on that how investigators or researchers are getting the performance of the reactors variance from the conventional reactors? So in that case, to increase the surface area and the internal fins or the main that aspects, to increase that that performance of the reactor and that is why that the geometry is the main factors to get that the performance of the reactor based on the creation of the surface area by that internal geometry.

And in this case, fins is one of the important geometrical effect where i can give a stabilising effect on the gas-liquid flow and allow the operation in countercurrent mode without flooding. So that is why, that internal fins are sometimes advisable to procure or design that reactor to get that the stabilising effect in the reactor. And hydrodynamics of such speciality monoliths will be different from that of the straight channel monoliths in that case. So these are the different geometrical effect on that performance of the monolithic reactors.

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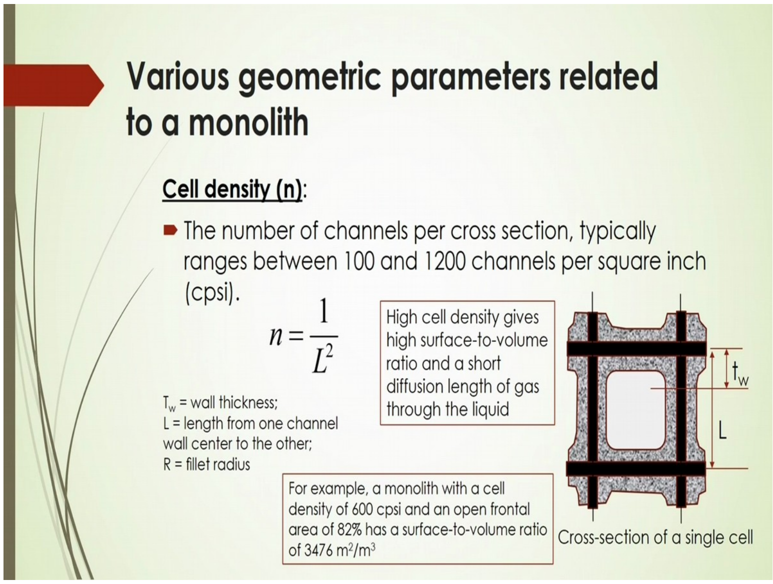

Various geometric parameters related to a monolith

Cell density (n):

- The number of channels per cross section, typically ranges between 100 and 1200 channels per square inch (cpsi).

$$n = \frac{1}{L^2}$$

High cell density gives high surface-to-volume ratio and a short diffusion length of gas through the liquid

T_w = wall thickness;
L = length from one channel wall center to the other;
R = fillet radius

For example, a monolith with a cell density of 600 cpsi and an open frontal area of 82% has a surface-to-volume ratio of 3476 m^2/m^3

Cross-section of a single cell

And you see that various geometric parameters that is related to the monolith here like we will see that if you are considering that channel based monolithic reactor there, you will see there will be certain that geometrical shape there, as shown in figure here some channels will be there, cross-section of a single cell will be there. In that case, the number of channels per cross sections, that will be typically ranges from 100 to 1200 per square inch, that is denoted by cpsi. So how to calculate that cpsi, that it is actually denoted by that *n* and it will be as 1 by L square as given in equation here in the slide

$$n = \frac{1}{L^2}$$

where this n is called that number of cell and L is called the length from one channel wall centre to the other there as per figure shown in the slides here.

So high cell density gives high surface to volume ratio and a short diffusion length of gas through the liquid which will be that suggested for the better performance of the monolithic reactor. For example, a monolith with a cell density of 600 cpsi and open frontal area of such as an example, 82 percent has a surface to volume ratio of 3476 meter square per meter cube. So you can say that if you increase that cell density, then you can have that more performance to get the that more surface to volume ratio there and you can get that more mass transfer for that particular chemical engineering processes. So you can get the more output of the either reactions or some other physical processes also.

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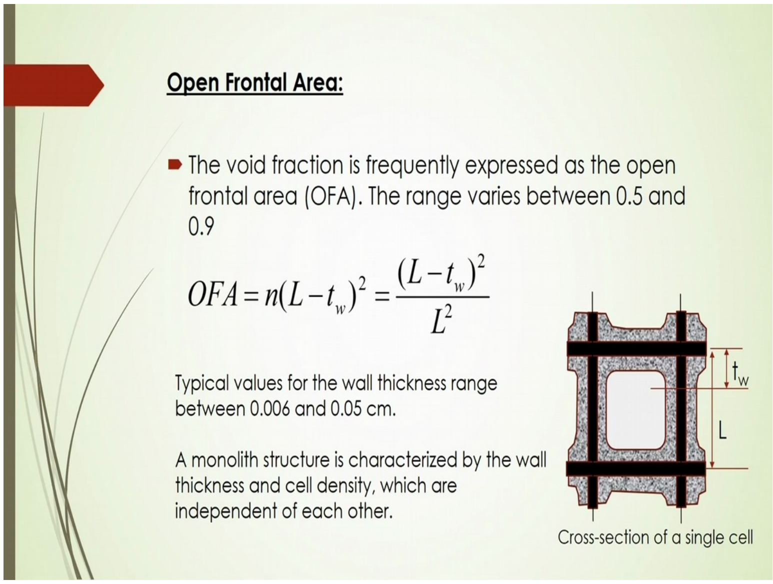

Open Frontal Area:

- The void fraction is frequently expressed as the open frontal area (OFA). The range varies between 0.5 and 0.9

$$OFA = n(L - t_w)^2 = \frac{(L - t_w)^2}{L^2}$$

Typical values for the wall thickness range between 0.006 and 0.05 cm.

A monolith structure is characterized by the wall thickness and cell density, which are independent of each other.

Cross-section of a single cell

Now what is that open frontal area, that is very important because the cell density, that depends on that open, that frontal area, that because this open frontal area will give you the measurement of the surface to volume ratio there. So the void fraction is frequently expressed as the open frontal area. The range that varies between 0.5 to 0.9, so we can represent this open frontal area as OFA. This is a function of a number of that cell and also what should be the length L and also width of that channel that is given there.

$$OFA = n(L - t_w)^2 = \frac{(L - t_w)^2}{L^2}$$

t_w, it is given here as shown in figure earlier slides that here t_w is nothing but the wall thickness here and L is called the length from one channel wall centre to the other. So it is a function of that L, t_w and n. So this open frontal area can be calculated from this equation given here that OFA is equal to $n(L - t_w)^2$. And that can be simplified upon substitution of this value of n from the previous equation that, then finally we can get that open frontal area will be equals to $n(L - t_w)^2$.

Typically, you can say the values for the wall thickness range is between 0.006 to that 0.005 centimeter. So in a monolithic structure is generally characterised by this wall thickness and the cell density which are independent of each other there. So you have to remember that though this cell density and this wall thickness are not related to each other, but it, these parameters will give you that void fraction that is called open frontal area which is actually directly influence the mass transfer coefficient for that particular chemical engineering process.

Any chemical engineering process whether it would be physical or chemical processes, there of course that mass transfer will happen either in with reactions or without reactions, then that mass transfer coefficient is related to this that geometry as well as that frontal area, that means here that void fraction of that particular phases which is passing through that cell. So that is why, cell structure, cell density, cell that cross-sectional area will be the geometrical effect for that particular chemical engineering process's output.

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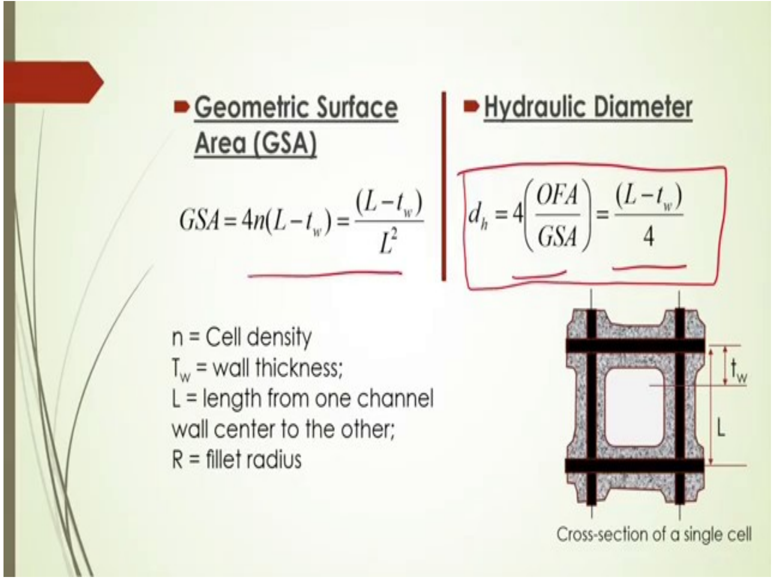

- **Geometric Surface Area (GSA)**

$$GSA = 4n(L-t_w) = \frac{(L-t_w)}{L^2}$$

n = Cell density
T_w = wall thickness;
L = length from one channel wall center to the other;
R = fillet radius

- **Hydraulic Diameter**

$$d_h = 4\left(\frac{OFA}{GSA}\right) = \frac{(L-t_w)}{4}$$

Cross-section of a single cell

Now geometric surface area, that is also important because how you will calculate that geometric surface area which is actually responsible for that particular that mass transfer between the surfaces. So that geometric surface area again, it will be a function of that number of cell density and also that wall thickness, length from one channel wall to the other and also one important factor here, that will be called as that fillet radius there because that fillet radius will give you that particularly what should be the that hydraulic diameter and based on that hydraulic diameter, you have to that analyse the frictional resistance as well as mixing characteristics and other operating characteristics of that monolithic reactor there. So geometric surface area can be calculated by this equation here.

$$GSA = 4n(L - t_w) = \frac{(L - t_w)}{L^2}$$

Whereas that hydraulic diameter, it will be as that 4 into OFA by GSA and it will be is equal to L minus t_w by 4 upon simplification. So you have to remember this, how to calculate that hydraulic diameter for this monolithic reactor. Once you know that L and t_w, then you can easily calculate what should be that hydraulic diameter,

$$d_h = 4\left(\frac{OFA}{GSA}\right) = \frac{(L - t_w)}{4}$$

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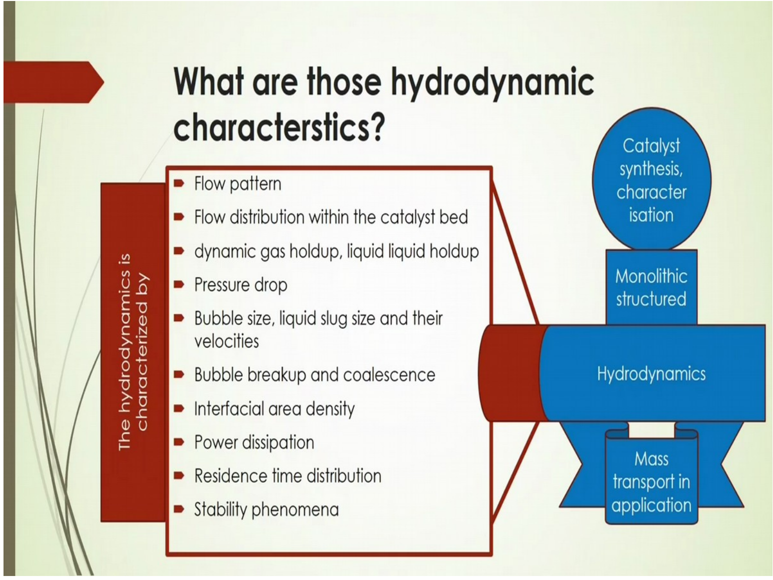

What are those hydrodynamic characterstics?

The hydrodynamics is characterized by

- Flow pattern
- Flow distribution within the catalyst bed
- dynamic gas holdup, liquid liquid holdup
- Pressure drop
- Bubble size, liquid slug size and their velocities
- Bubble breakup and coalescence
- Interfacial area density
- Power dissipation
- Residence time distribution
- Stability phenomena

Now what are those hydrodynamic characteristics? That I told that several hydrodynamic characteristics that actually affect the performance of the reactor. So first one is that flow pattern, there are several different types of flow patterns. We know that for gas- liquid operation, we know that plug flow, slug flow, bubbly flow, even annular flow, even we can say that stratified flow, there are several different types of flow patterns. And for liquid-liquid also, we are getting different types of flow patterns there and gas-liquid-solids three-phase also, we are getting that churn-turbulent homogeneous slug flow, plug flow and you know that particulate flow, there are different types of flow patterns.

So those flow patterns actually will give you that different types of mass transfer efficiency, even reaction performance and then overall, that reactor efficiency for that particular chemical engineering processes. And also, another important hydrodynamic characteristics, the flow distribution within that catalyst bed. Since that monolithic reactor is nothing but that bed of the catalyst as a channel or surface with a particular structure, so how that you know flow will be distributed through the channel that should be the important factor for the analysis or performance of the reactor.

And another thing is the dynamic gas hold-up. Whenever gas-liquid reactions would be carried out through this reactor, then what should be the hold-up of that gas? What should be the liquid-liquid hold-up there inside the reactor, that also to be important to be noted down because those things also directly or indirectly related to that performance of the reactor. And pressure drop is another important factor, at a particular pressure that whenever reactions or that mass transfer characteristics would be carried out, that you have to know that how the flow will be getting that resistance through the reactor that may that effect on the mass transfer characteristics.

Again, if you are considering that gas-liquid flow through the channel, there may be that bubble slug or gas slug, liquid slug. So in that case, you have to know the size of that particular slug. That slug maybe you can say that bubble slug or bubble size in that case and also liquid slug size and their velocities how actually those slug will be flowing through the channel that should be actually considered to study. And also, if the bubbles are forming there inside the channels, then how it will be breakup and how it may be collisions to get that elongated bubble size there?

So that also to be considered as a hydrodynamic characteristic. And then interfacial area density also, through that monolithic channel for particular volume that what should be the surface area which is taking part for that particular reactions or chemical engineering processes, that you have to calculate as a density, that is interfacial area density. And also power dissipation is important. What would be the consumption of the power that also to be considered because the performance of the chemical engineering processes in that particular reactors should be economic.

So what will be the power dissipation, that also to be considered as a hydrodynamic characteristics here? And residence time distribution, of course, that is very important. You know the how long that phase will be residing through the channel for that particular chemical engineering processes whenever that gas-liquid reactions or liquid-liquid reactions or gas-liquid-solid reactions there in presence of this monolithic catalyst. So in that case residence time of the each phases should be, are required to know.

And also stability phenomena, whether this monolithic structures are stable or not? So that is why, these are the different hydrodynamic characteristics which is very important to know for getting the performance of the reactor and also that different aspects of the reactor for designing of that particular structure based on these hydrodynamic characteristics. Now so what is to know that based on the hydrodynamic characteristics, you have to pass the catalyst synthesis and characterisation after that monolithic structure to be procured, that already we have discussed, to procure that monolithic structure.

And also after procurement of that monolithic structure that you have to study the different hydrodynamic characteristics based on which you have to analyse the mass transfer characteristics of that particular reactor and upon which you will be able to that say what will be the efficiency of that reactor for that particular processes.

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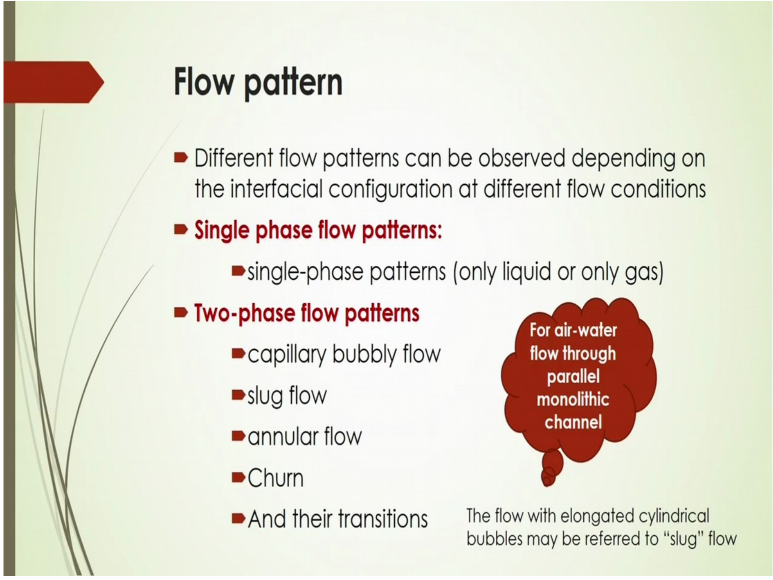

Flow pattern

- Different flow patterns can be observed depending on the interfacial configuration at different flow conditions
- **Single phase flow patterns:**
    - single-phase patterns (only liquid or only gas)
- **Two-phase flow patterns**
    - capillary bubbly flow
    - slug flow
    - annular flow
    - Churn
    - And their transitions

For air-water flow through parallel monolithic channel

The flow with elongated cylindrical bubbles may be referred to “slug” flow

Now we will discuss something about that flow pattern hydrodynamics there. So different flow patterns we have told that can be observed depending on the interfacial configuration at a different flow conditions. And now single phase flow pattern sometimes it has happened in the structured reactor like single phase patterns, only liquid or only gas may be there, liquid slug will be there or only single liquid will be flowing without making any slug there. And also, 2 phase flow patterns there, you can have that capillary bubble slug, slug flow of the liquid, even also annular flow.

That means in core regions, there will be a one phase and then the wall regions, there will be another liquid there. So there the annular flow will be there. Churn flow, there will be intermixing of the fluid particles at higher flow rate. Then, churning of that phases will be happening, so it is called churn turbulent flow. And then also, other factors, it is called transition, whether it may be that annular or slug particularly that transition it may either slug or annular. So in that particular operating conditions, you may get that slug and annular both mixed there in a particular operating conditions. So that is called transitions.

So for air-water flow through the parallel monolithic channel, you are having this type of that flow patterns like capillary, slug, annular, churn and their transitions.

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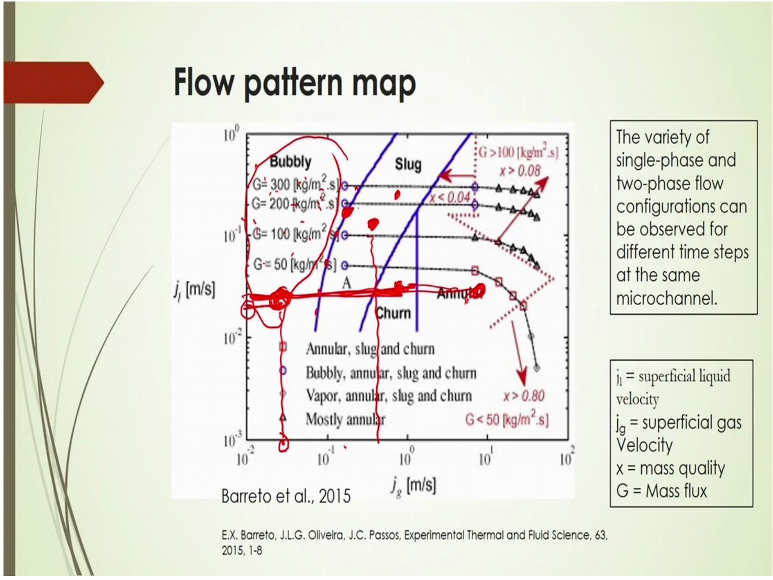

Flow pattern map

The variety of single-phase and two-phase flow configurations can be observed for different time steps at the same microchannel.

j_l = superficial liquid velocity
j_g = superficial gas Velocity
x = mass quality
G = Mass flux

E.X. Barreto, J.L.G. Oliveira, J.C. Passos, Experimental Thermal and Fluid Science, 63, 2015, 1-8

And here one typical flow pattern map is shown there as per, Barreto et al., they have actually given this flow pattern for this monolithic reactor. They have published this data in experimental thermal and fluid sciences in 2015. As per their experimental observations, they have concluded that the variety of single phase and two phase flow configurations can be observed for the different time steps of the same micro-channel of monolithic structure. And they have actually made one flow pattern map. Flow pattern map, what is that? This is nothing but the graphical representation of the transition of different flow pattern that is observed in that particular channel.

So that things are actually represented in a graph. That is called flow pattern map. Now in this flow pattern map, we are considering that there will be X axis is here, JG means here superficial gas velocity and JL which is denoted for superficial liquid velocity. So if there is a gas-liquid operations through that monolithic microstructure reactor, you will see that at various that gas and liquid velocity, you may have different types of flow patterns there. So if you increase the gas flow rate by keeping your liquid velocity constant, then you may have flow patterns from bubbly to slug or slug to churn or churn to annular flow.

Whereas in the opposite way also you can have those things like that if you increase the superficial liquid velocity by keeping your gas velocity there, then you can have this sometimes that churn turbulent flow to the slug flow, even to the bubbly flow. Even from it the annular flow also. So from this map, we are having different that data at different points, at different operating conditions and here you will see that blue line is actually showing that transition data where the transitions are from that from bubbly to slug or slug to churn or churn to annular.

So if you are considering a particular point here in the graph like here, you will see that at this point what we are getting here, what will be the that gas velocity and what will is the liquid velocity there? So at this point, at this gas velocity and at this liquid velocity, if you operate those monolithic reactors, you may get at this bubbly flow of pattern there. Even if you keep this gas velocity constant and if you increase the liquid velocity up to this, then you may get again that bubbly flow pattern. Again in this way if you are keeping your gas velocity constant and liquid velocity increasing, then you may have this region of this bubbly flow pattern.

So at any point of this region, that means at the combination at the point of this J_G and J_L, then you may expect that it will be a bubbly flow regime. Whereas at this location, if you consider a point here, what will happen here? The gas velocity is a little bit higher and also, from this point, liquid velocity is a little bit higher. So at higher gas velocity and liquid velocity compared to this previous point of this bubbly flow, you may expect that slug flow. So this slug flow, it will happen here at this combination.

You may get this slug flow here itself also. In this point also, what should be the gas velocity? Little bit higher and also liquid velocity also little bit higher. But in this case also, you may get the slug flow. But if you consider the point here, this is the transition where at this gas and liquid velocity you may get the optimum value or you get the maximum value of this gas velocity and where you may change the liquid velocity so that you can get this bubbly flow to that slug flow regime. So here, this is the point. These are the point from which you can say at this particular operating condition of gas and liquid velocity, you may get that transition of this bubbly to slug flow.

Similarly, again if you increase the gas velocity from this that from this point to this, you may expect this at the same constant liquid velocity as earlier, at higher gas velocity, you may get the churn turbulent flow instead of slug flow. Even if you increase that gas velocity and if you consider the point here, you may get that liquid velocity. So in this way, by just getting that data point of that gas and liquid velocity and considering that you may get that, you may expect or speculate what type of flow pattern will be there. So this flow pattern map will give you that you know that expected flow pattern during your operation. So before going to experiment, to study different hydrodynamic characteristics, then you have to that fix a certain gas and liquid velocity for that particular that chemical engineering process.

That process may be feasible in the slug flow, that process may be feasible in bubbly flow, so accordingly, you have to select that particular gas flow rate and liquid flow rate to get that particular flow pattern. So that can be obtained by this flow pattern map. So this is the importance to study this flow pattern map and also this you have to utilise for that study of different hydrodynamic characteristics and mass transfer characteristics based on the flow pattern. So I think it will be very helpful for your analysis of chemical engineering process based on the flow pattern and also what should be the particular operating conditions there.

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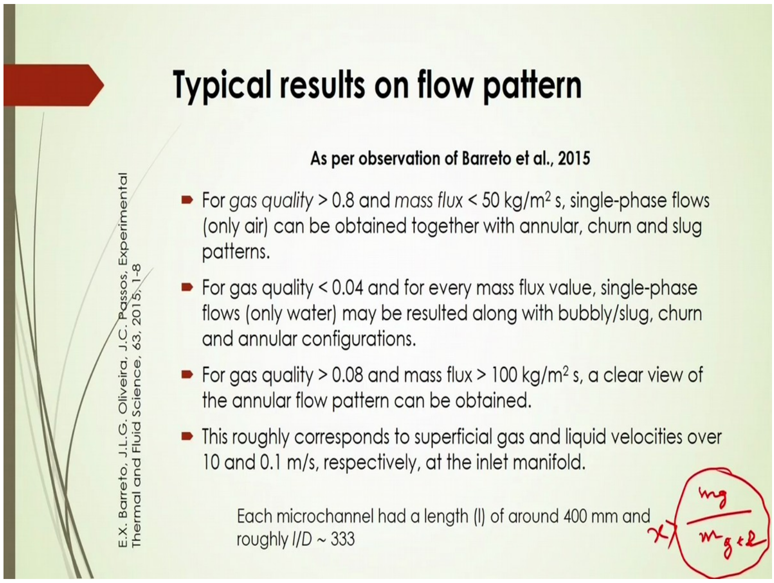

Typical results on flow pattern

As per observation of Barreto et al., 2015

- For *gas quality* > 0.8 and *mass flux* < 50 kg/m^2 s, single-phase flows (only air) can be obtained together with annular, churn and slug patterns.
- For gas quality < 0.04 and for every mass flux value, single-phase flows (only water) may be resulted along with bubbly/slug, churn and annular configurations.
- For gas quality > 0.08 and mass flux > 100 kg/m^2 s, a clear view of the annular flow pattern can be obtained.
- This roughly corresponds to superficial gas and liquid velocities over 10 and 0.1 m/s, respectively, at the inlet manifold.

Each microchannel had a length (l) of around 400 mm and roughly l/D ~ 333

$x > \frac{m_g}{m_{g+l}}$

E.X. Barreto, J.L.G. Oliveira, J.C. Passos, Experimental Thermal and Fluid Science, 63, 2015, 1-8

Now typical results on flow pattern like for gas quality is greater than 0.1. What is that gas quality is also important factor. In this case gas quality means what is the mass ratio of that gas to the mass of the liquid there, mass of the gas and liquid mixture there. So that is called gas quality. That means mass of gas divided by total mass of gas and liquid. Total mass of gas and liquid if is there a gas and liquid mixture flowing through the channel. So in that case, gas quality will be considered like this. So this is called gas quality. So if this gas quality, it is denoted by x, is greater than 0.8 and mass flux, that means velocity into density, if it is 50 kg per meter square second, then you may expect that only single phase flow, that is only air. And in that case that you may expect along with that single phase flow with annular churn and slug patterns.

So for gas quality, if it is less than 0.04 and for every mass flux value, single phase flows only water, may be resulted along with bubbly or slug, churn and annular configurations. And for gas quality if it is greater than 0.08 and mass flux if it is greater than 100 kg per meter square second, a clear view of the annular flow pattern can be obtained. And this actually roughly corresponds to the superficial gas and liquid velocities over 10 and 0.1 meter per second respectively at the inlet manifold in the monolithic structure.

So you actually can optimize on which gas quality to be maintained to get that particular flow pattern. So these are observations based on that experimental results, actually obtained by Baretto et al. in 2015.

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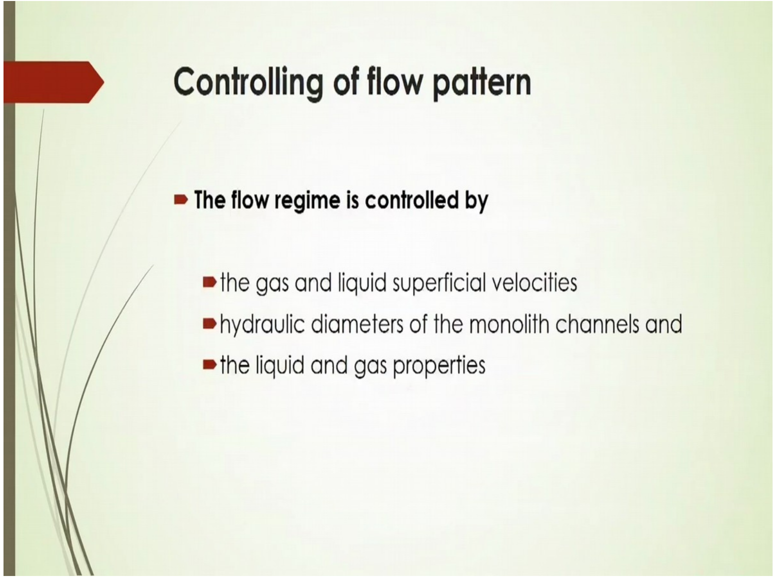

Controlling of flow pattern

- The flow regime is controlled by
  - the gas and liquid superficial velocities
  - hydraulic diameters of the monolith channels and
  - the liquid and gas properties

Now how to control those flow patterns? The flow regimes can be, flow regime, sometimes flow pattern it is called flow regime. So this flow regime can be controlled by that gas and liquid superficial velocities, hydraulic diameters of the monolithic channels and the liquid and gas properties.

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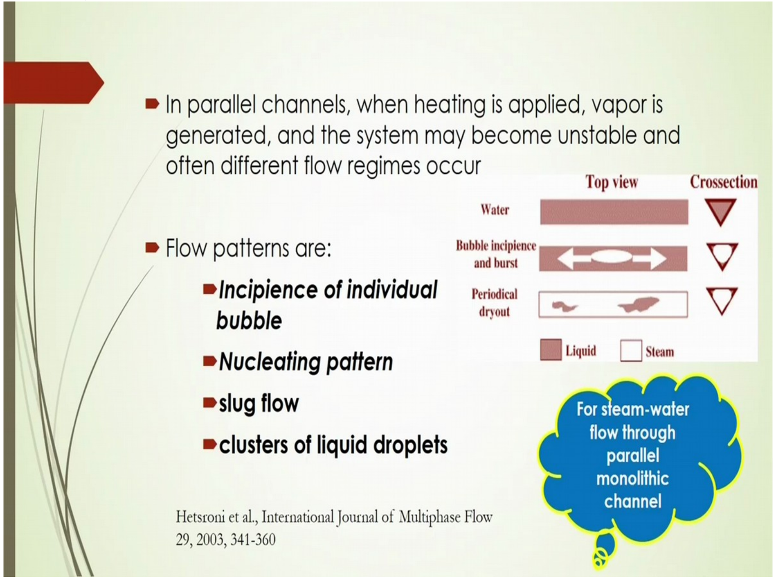

- In parallel channels, when heating is applied, vapor is generated, and the system may become unstable and often different flow regimes occur
- Flow patterns are:
  - ***Incipience of individual bubble***
  - ***Nucleating pattern***
  - **slug flow**
  - **clusters of liquid droplets**

For steam-water flow through parallel monolithic channel

Hetsroni et al., International Journal of Multiphase Flow 29, 2003, 341-360

In the parallel channels, when heating is applied, vapor is generated and in that case the system may become unstable and often you can get different types of flow patterns or regimes. And in that case, you may expect the flow pattern of incipience of individual bubble, nucleating pattern, slug flow, or clusters of liquid droplets. And this is reported by Hetsroni et al., in 2003. They have published their work in the International Journal of Multiphase Flow in 2003. So for stream water flow through the parallel monolithic channel, you may expect this incipience of individual bubble, nucleating pattern, even slug flow, clusters of liquid droplets, these are the different flow patterns you can expect in this particular type of channel.

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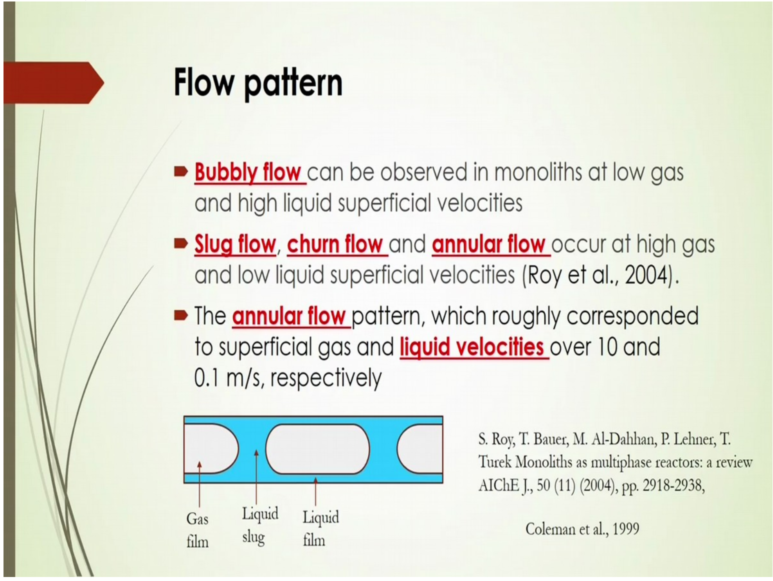

Flow pattern

- **Bubbly flow** can be observed in monoliths at low gas and high liquid superficial velocities
- **Slug flow**, **churn flow** and **annular flow** occur at high gas and low liquid superficial velocities (Roy et al., 2004).
- The **annular flow** pattern, which roughly corresponded to superficial gas and **liquid velocities** over 10 and 0.1 m/s, respectively

S. Roy, T. Bauer, M. Al-Dahhan, P. Lehner, T. Turek Monoliths as multiphase reactors: a review AIChE J., 50 (11) (2004), pp. 2918-2938,

Coleman et al., 1999

Now flow pattern or other also may be happened that depends on that geometry of that channel. So bubbly flow can be observed in monoliths at low gas and high liquid superficial velocities. Slug flow, churn flow and annular flow that may occur at high gas and low liquid superficial velocities as per Roy et al., in 2004. They have actually published their experimental work and observations for that flow pattern study in monolithic structure and also the annular flow pattern which roughly corresponded to the superficial gas and liquid velocities over 10 and 0.1 meter per second respectively. That is also observed by that Coleman et al., 1999, that is reported in that in the review paper published by Roy et al. in 2004.

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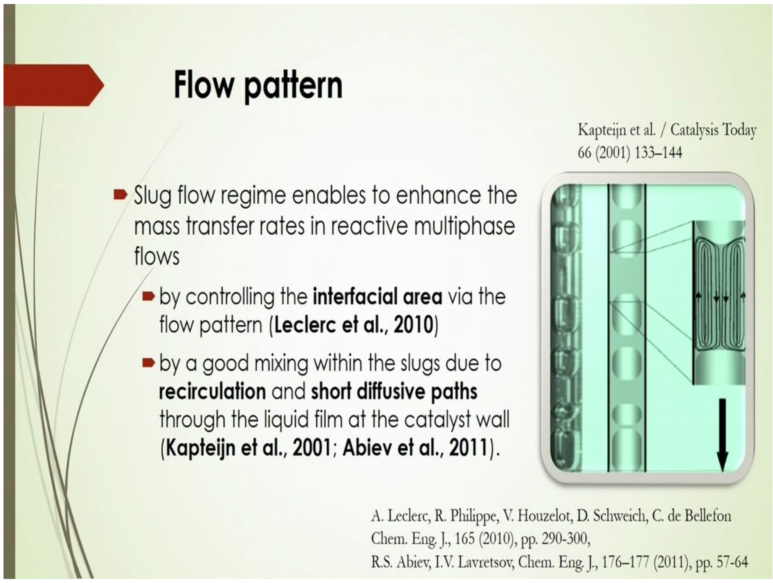

Flow pattern

Kapteijn et al. / Catalysis Today 66 (2001) 133–144

- Slug flow regime enables to enhance the mass transfer rates in reactive multiphase flows
  - by controlling the **interfacial area** via the flow pattern (**Leclerc et al., 2010**)
  - by a good mixing within the slugs due to **recirculation** and **short diffusive paths** through the liquid film at the catalyst wall (**Kapteijn et al., 2001**; **Abiev et al., 2011**).

A. Leclerc, R. Philippe, V. Houzelot, D. Schweich, C. de Bellefon Chem. Eng. J., 165 (2010), pp. 290-300,
R.S. Abiev, I.V. Lavretsov, Chem. Eng. J., 176–177 (2011), pp. 57-64

Flow pattern also that enables to enhance the mass rates in the reactive multiphase flow. Especially slug flow regimes are very important in this case. In that case, by controlling the interfacial area via the flow pattern, you can enhance the mass transfer rates as per Leclerc et al., in 2010 and also you may expect the enhancement of the mass transfer rates in reactive multiphase flows in case of that mixing characteristics where a good mixing within the slugs due to the recirculation and short diffusive path through the liquid film at the catalyst wall. That is actually given by Kapteijn et al., 2001 and Abiev et al., in 2011.

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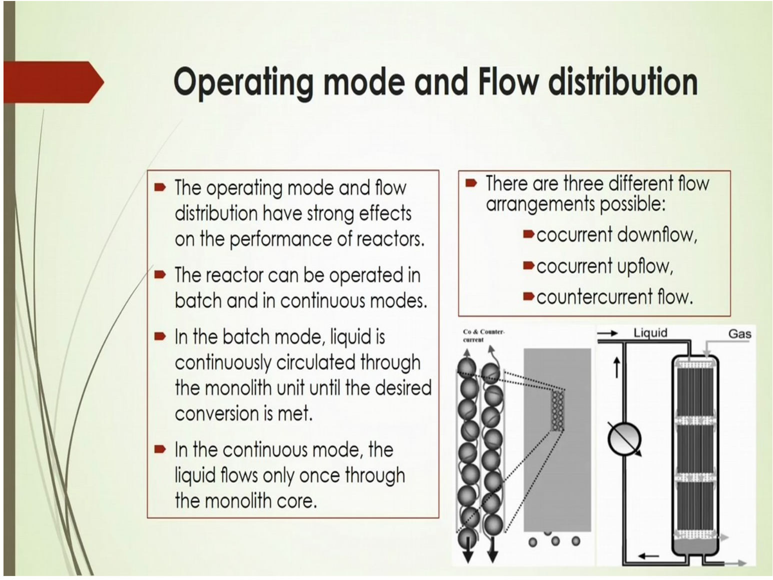

Operating mode and Flow distribution

- The operating mode and flow distribution have strong effects on the performance of reactors.
- The reactor can be operated in batch and in continuous modes.
- In the batch mode, liquid is continuously circulated through the monolith unit until the desired conversion is met.
- In the continuous mode, the liquid flows only once through the monolith core.

- There are three different flow arrangements possible:
  - cocurrent downflow,
  - cocurrent upflow,
  - countercurrent flow.

And there are several operating mode and flow distributions are observed in the monolithic structure reactor where you can say that the operating mode and flow distribution have the strong effects on the performance of reactors. The reactor can be operated in batch and in continuous modes. In the batch mode, liquid is continuously circulated through the monolith unit until the desired conversion is met. And in the continuous mode, the liquid flows only once through the monolith core is there.

So there are three different flow arrangements possible in that case: Co-current down flow, co-current upflow and the countercurrent flow. So there are different that operating mode and the flow distributions are happens in that in monolithic structure reactor.

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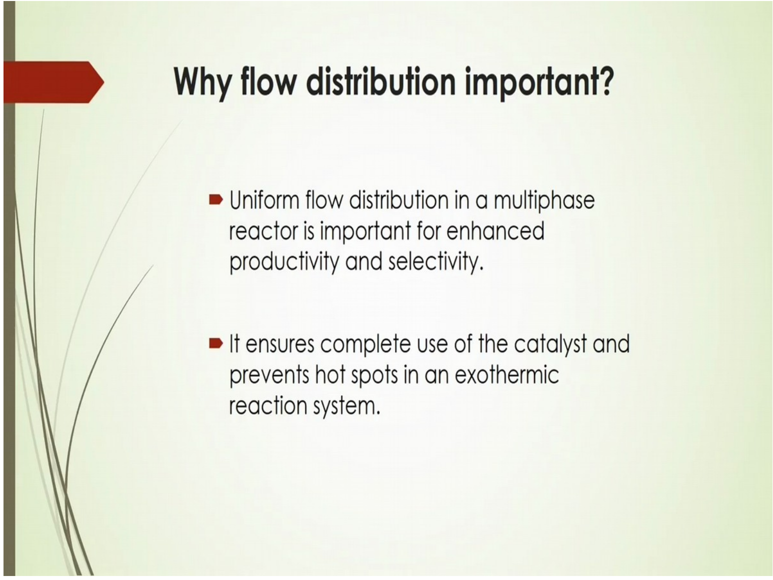

Why flow distribution important?

- Uniform flow distribution in a multiphase reactor is important for enhanced productivity and selectivity.
- It ensures complete use of the catalyst and prevents hot spots in an exothermic reaction system.

Now question is that, why you have to know that flow distribution in the monolithic reactor? Because the uniform flow distribution in the multiphase flow reactor is very important for enhancement of the productivity and selectivity. It generally ensures complete use of catalyst and prevents hot spots in an exothermic reaction system. So that is why, you have to know the flow distribution whether liquid is distributed properly or not, whether there is any that stagnation of that liquid in the channel or not, that stagnant region may sometimes hinder that performance of the reaction and also that may that reduce the intensity of the mixing inside the reactor for which that mass transfer will be reduced.

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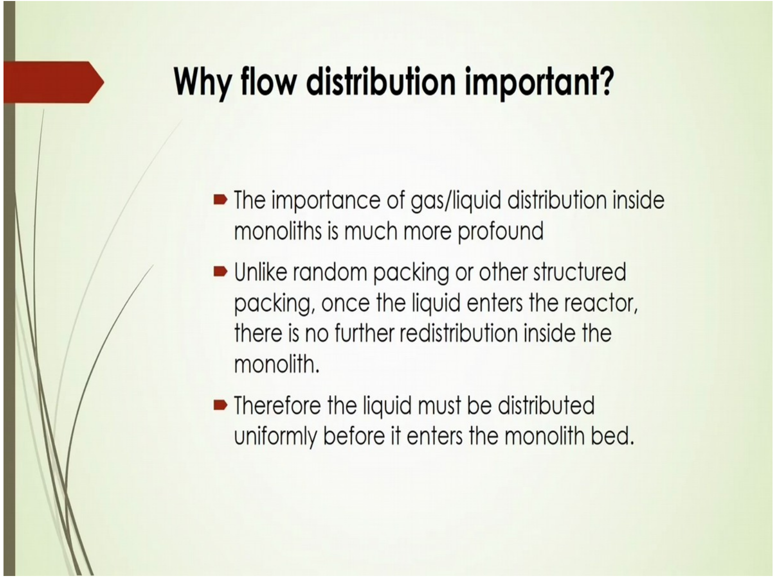

Why flow distribution important?

- The importance of gas/liquid distribution inside monoliths is much more profound
- Unlike random packing or other structured packing, once the liquid enters the reactor, there is no further redistribution inside the monolith.
- Therefore the liquid must be distributed uniformly before it enters the monolith bed.

So the importance of gas and liquid distribution inside the monolith is much more profound and which is to be that analysed and unlike random packing or other structured packing, once the liquid enters the reactor there is no further redistribution inside the monolith reactor. That is, as per that structured packing, therefore the liquid must be distributed uniformly before it enters the monolithic bed.

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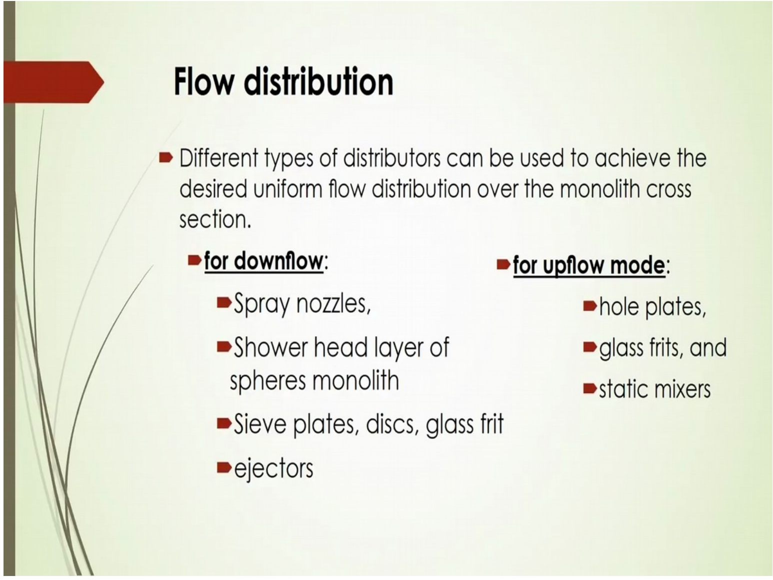

Flow distribution

- Different types of distributors can be used to achieve the desired uniform flow distribution over the monolith cross section.
  - **for downflow**:
    - Spray nozzles,
    - Shower head layer of spheres monolith
    - Sieve plates, discs, glass frit
    - ejectors
  - **for upflow mode**:
    - hole plates,
    - glass frits, and
    - static mixers

Now different types of distributors, sometimes we use to achieve those desired uniform flow distribution over the monolith cross-section. Like for downflow, for upflow mode what are the different distributors are being used for the distribution of the phases in the reactor. For the downflow generally, spray nozzles, showerhead layer of spheres monolith, even sieve plates, discs, glass frit, ejectors, these are the different distributors are being used for the distribution of the liquid. And for upflow, hole plates, that glass frits and static mixers are being used for that flow distribution of the liquid through the monolithic reactor.

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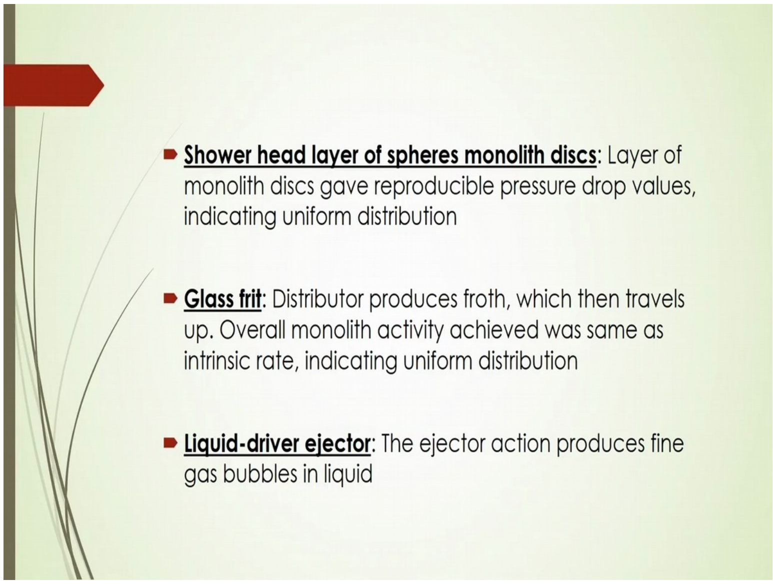

- **Shower head layer of spheres monolith discs**: Layer of monolith discs gave reproducible pressure drop values, indicating uniform distribution
- **Glass frit**: Distributor produces froth, which then travels up. Overall monolith activity achieved was same as intrinsic rate, indicating uniform distribution
- **Liquid-driver ejector**: The ejector action produces fine gas bubbles in liquid

Showerhead layer of spheres monolith discs, generally it is a layer of monolith disc that actually give the reproducible pressure drop values, indicating uniform distribution. Whereas glass frit distributor produces froth, which then travels up and overall monolith activity achieved may be same as intrinsic rate that will indicate the uniform distribution. In case of liquid-driver ejector type of distributor, the ejector action produces fine gas bubbles in the liquid which may be easier to distribute throughout the channel to get that more interfacial area between gas and liquid to get more mass transfer efficiency in that particular chemical engineering process.

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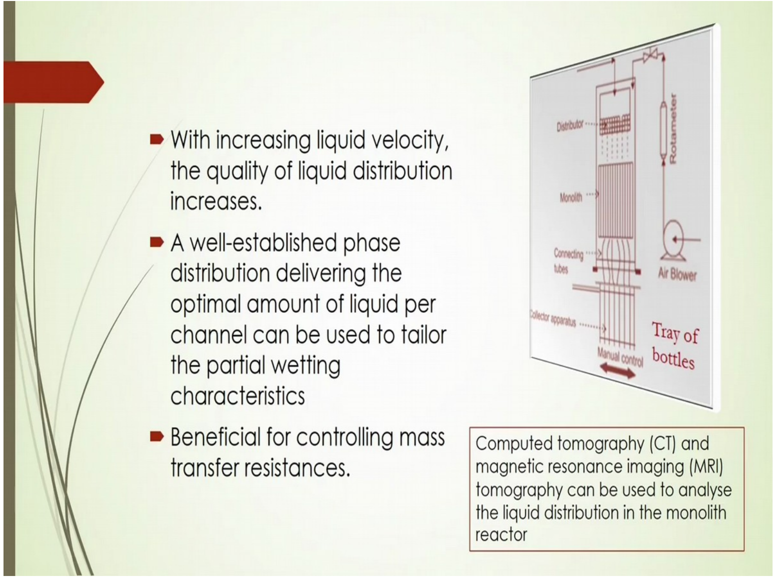

- With increasing liquid velocity, the quality of liquid distribution increases.
- A well-established phase distribution delivering the optimal amount of liquid per channel can be used to tailor the partial wetting characteristics
- Beneficial for controlling mass transfer resistances.

Computed tomography (CT) and magnetic resonance imaging (MRI) tomography can be used to analyse the liquid distribution in the monolith reactor

Now with increasing liquid velocity, sometimes the quality of the liquid distribution increases but sometimes it may be decreased because of that design of that channel. If you have designed that channel with some internals to get that more mixing there, that may sometimes give you that static region of that liquid. So generally, increasing liquid velocity, the quality of liquid distribution increases. But if there is a special structure where that you are actually inserting some internal, there sometimes it may give you that some stagnant region.

So if you are optimising those stagnation factor for the liquid distribution, then you can get that enhancement of the mass transfer based on this liquid distribution. A well-established face distribution delivering the optimal amount of liquid per channel, that can be used to tailor the partial wetting characteristics sometimes. So you know that you have to design that reactor via that phase distribution, maybe optimal amount of liquid through that channel and for the characterizing the partial wetting there during the flow distribution.

And beneficial for the controlling mass transfer resistance are most important because that depends on that flow characteristics like flow distribution through the channel. So that is why that flow distribution is one of the important beneficial factor for controlling mass transfer resistances. And this flow distribution, how you will actually estimate experimentally, you may or you can use that computed tomography system, magnetic resonance imaging system for the observation of the liquid distribution in the channel and you can analyse it by different that suitable model to predict that particular intensity of the distribution of the liquid inside the reactor.

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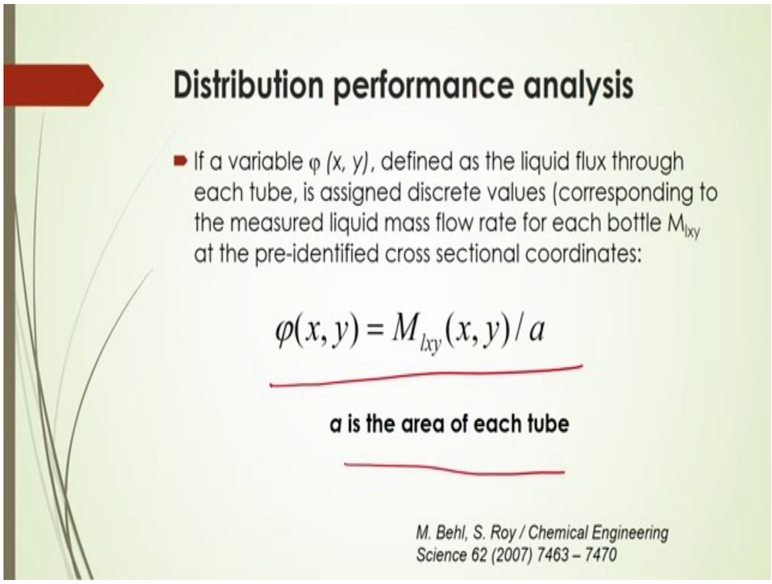

Distribution performance analysis

- If a variable φ (x, y), defined as the liquid flux through each tube, is assigned discrete values (corresponding to the measured liquid mass flow rate for each bottle M_{lxy} at the pre-identified cross sectional coordinates:

$$\varphi(x,y) = M_{lxy}(x,y)/a$$

a is the area of each tube

M. Behl, S. Roy / Chemical Engineering Science 62 (2007) 7463 – 7470

Now then distribution performance analysis, how you will do based on that distribution of the liquid? If a variable if you consider that φ which is a function of x and y,

$$\varphi(x,y) = M_{lxy}(x,y)/a$$

if it is defined as the liquid flux through each tube and it is designed discrete values, and it is assigned to discrete values corresponding to the measured liquid mass flow rate for each bottle, bottle means here where that liquid is collected after distributing or it is coming out from the reactor at a free identified cross-sectional coordinates, then you can have this situation like this φ in the x and y direction, it will be a function of mass flow rate liquid, liquid that is, liquid mass flow rate which is coming out from the reactor after distribution. So by this equation, you can actually analyse those performance of the distribution. In this case, a is called that area of each tube or channel in the reactor. So this equation, this concept is given by Behl and Roy in 2007.

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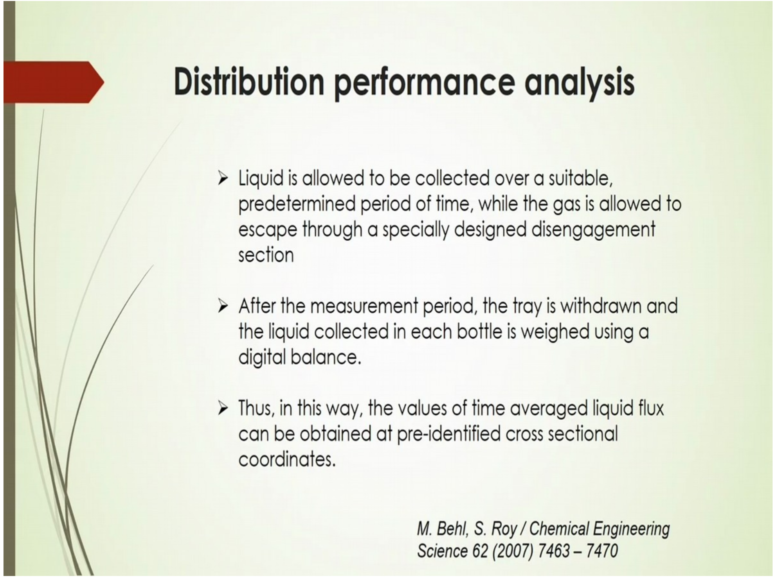

Distribution performance analysis

- Liquid is allowed to be collected over a suitable, predetermined period of time, while the gas is allowed to escape through a specially designed disengagement section
- After the measurement period, the tray is withdrawn and the liquid collected in each bottle is weighed using a digital balance.
- Thus, in this way, the values of time averaged liquid flux can be obtained at pre-identified cross sectional coordinates.

M. Behl, S. Roy / Chemical Engineering Science 62 (2007) 7463 – 7470

And according to their observation that and also their that concept that liquid is allowed to be collected over a suitable, predetermined period of time while the gas is allowed to escape through especially designed disengagement section. After the measurement period, the tray should be withdrawn and the liquid collected in each bottle is weighted using a digital balance. After that you can analyse those values of time average liquid flux that is obtained at pre-identified cross-sectional coordinates.

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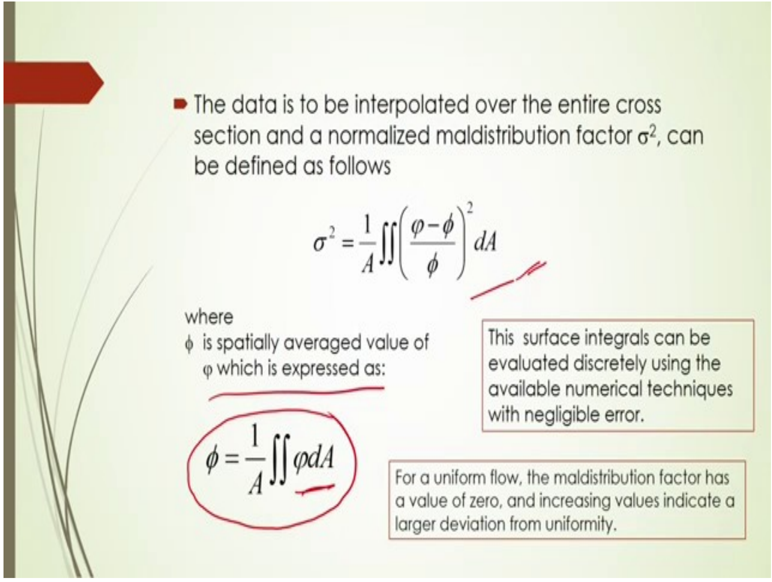

- The data is to be interpolated over the entire cross section and a normalized maldistribution factor σ^2, can be defined as follows

$$\sigma^2 = \frac{1}{A}\iint\left(\frac{\varphi-\phi}{\phi}\right)^2 dA$$

where
ϕ is spatially averaged value of φ which is expressed as:

$$\boxed{\phi = \frac{1}{A}\iint \underline{\varphi dA}}$$

This surface integrals can be evaluated discretely using the available numerical techniques with negligible error.

For a uniform flow, the maldistribution factor has a value of zero, and increasing values indicate a larger deviation from uniformity.

And then data is to be incorporated over the entire cross-section and a normalised maldistribution factor to be defined such as here it is given here,

$$\sigma^2 = \frac{1}{A}\iint\left(\frac{\varphi - \phi}{\phi}\right)^2 dA$$

as shown in equation here in the slides, where phi is specially averaged value of that phi here which is expressed as like this. So this ϕ is equal to

$$\phi = \frac{1}{A}\iint \varphi dA$$

So in this case, the surface integrals can be evaluated discreetly using the available numerical techniques with negligible error and for a uniform flow, the maldistribution factor has a value of 0 and the increasing values indicate a larger deviation from the uniformity.

So you have to remember these things that when this maldistribution or what should be the maldistribution factor and if it is coming to 0, then you can get that uniform flow.

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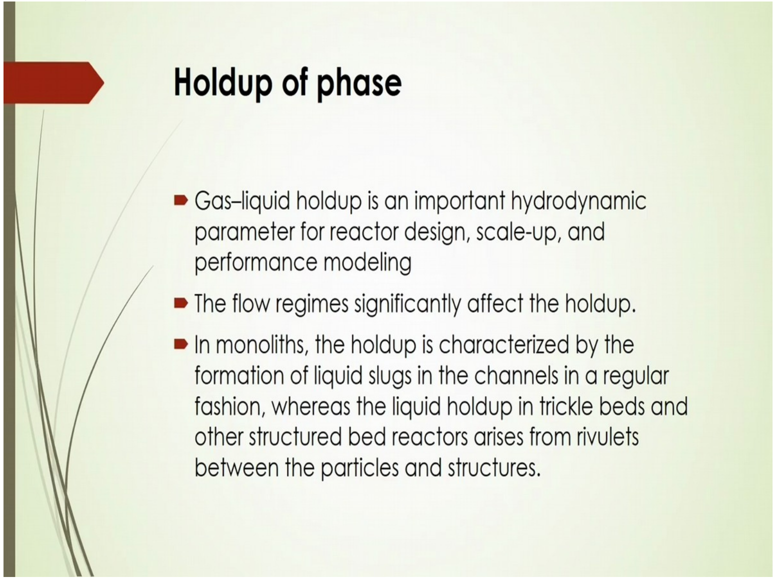

Holdup of phase

- Gas–liquid holdup is an important hydrodynamic parameter for reactor design, scale-up, and performance modeling
- The flow regimes significantly affect the holdup.
- In monoliths, the holdup is characterized by the formation of liquid slugs in the channels in a regular fashion, whereas the liquid holdup in trickle beds and other structured bed reactors arises from rivulets between the particles and structures.

Next one of the important that hydrodynamic factor it is called the holdup of the phases. What is that hold-up of the phases? Now if you are considering the two-phases like gas and liquid, then what will be the volume of that individual phase that is occupied in that particular channel of that reactor? It is called that hold-up of the phases. If you are considering gas-liquid hold-up in an important gas liquid system, then hold-up is an important hydrodynamic parameter for that reactor design, scale up and performance modelling. And in this case, this flow regime that depends on this hold-up of that gas-liquid system.

And in monoliths, the hold-up is characterised by the formation of liquid slugs in the channels in a regular fashion, whereas the liquid hold-up in the trickle beds and others structured bed reactors arises from rivulets between the particles and the structures. So this is the difference of that hold-up structure or characteristic factors in the monolithic channel and the trickle bed reactor.

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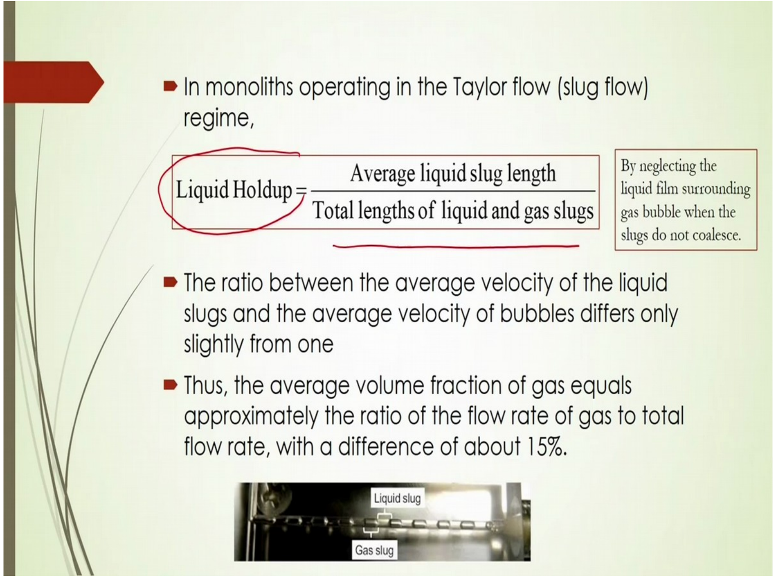

- In monoliths operating in the Taylor flow (slug flow) regime,

$$\text{Liquid Holdup} = \frac{\text{Average liquid slug length}}{\text{Total lengths of liquid and gas slugs}}$$

By neglecting the liquid film surrounding gas bubble when the slugs do not coalesce.

- The ratio between the average velocity of the liquid slugs and the average velocity of bubbles differs only slightly from one
- Thus, the average volume fraction of gas equals approximately the ratio of the flow rate of gas to total flow rate, with a difference of about 15%.

In the monoliths operating in the Taylor flow that is called slot flow regime, in that case that liquid hold-up you can calculate by this equation where you can get it from the average liquid slug length and also total lengths of the liquid and gaseous slugs. So in this case you have to neglect the liquid film that is surrounded to the gas bubbles when the slugs do not coalesce there. So the ratio between the average velocity of the liquid slugs and the average velocity of the bubbles differs only slightly from one there in the slug flow pattern in the monolithic channel, that is why you can directly obtain those liquid hold-up from this that slug length and the gaseous slug length.

So average volume fraction of the gas that will, equals approximately the ratio of the flow rate of the gas to the total flow rate with a difference of about 15 percent. So either you can get it from the slug length of the gas and liquid or you can get it from the velocities of the gas and liquid through the channel.

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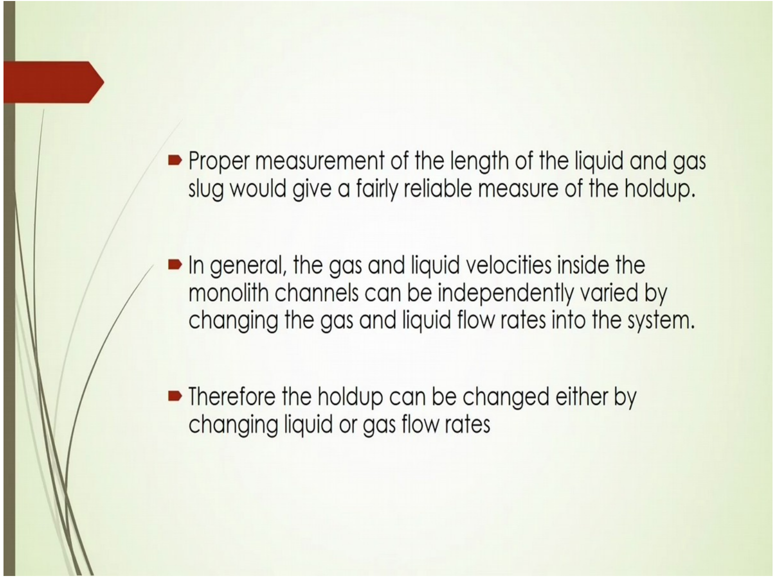
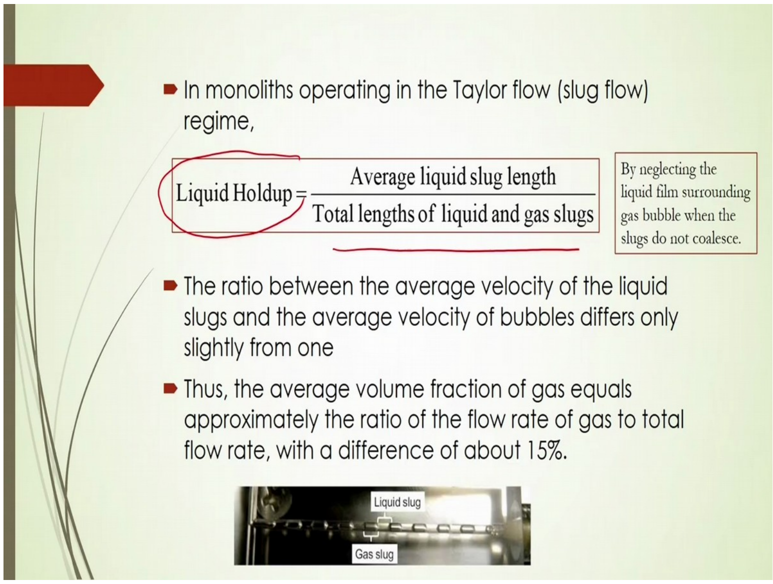


- Proper measurement of the length of the liquid and gas slug would give a fairly reliable measure of the holdup.
- In general, the gas and liquid velocities inside the monolith channels can be independently varied by changing the gas and liquid flow rates into the system.
- Therefore the holdup can be changed either by changing liquid or gas flow rates



- In monoliths operating in the Taylor flow (slug flow) regime,

$$\text{Liquid Holdup} = \frac{\text{Average liquid slug length}}{\text{Total lengths of liquid and gas slugs}}$$

By neglecting the liquid film surrounding gas bubble when the slugs do not coalesce.

- The ratio between the average velocity of the liquid slugs and the average velocity of bubbles differs only slightly from one
- Thus, the average volume fraction of gas equals approximately the ratio of the flow rate of gas to total flow rate, with a difference of about 15%.

Proper measurement of the length of the liquid and gas slugs would give a fairly reliable measurement of the hold-up based on this equation. In general, the gas and liquid velocity inside the monolith channel that can be independently varied by changing the gas and liquid flow rates into the system. Therefore, the hold-up can be changed either by changing liquid or gas flow rates.

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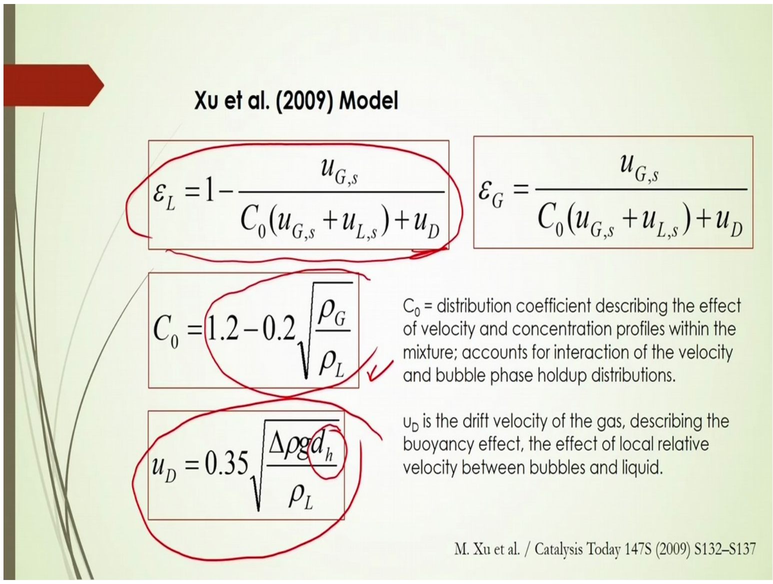

Xu et al. (2009) Model

$$\varepsilon_L = 1 - \frac{u_{G,s}}{C_0(u_{G,s}+u_{L,s})+u_D}$$

$$\varepsilon_G = \frac{u_{G,s}}{C_0(u_{G,s}+u_{L,s})+u_D}$$

$$C_0 = 1.2 - 0.2\sqrt{\frac{\rho_G}{\rho_L}}$$

C_0 = distribution coefficient describing the effect of velocity and concentration profiles within the mixture; accounts for interaction of the velocity and bubble phase holdup distributions.

$$u_D = 0.35\sqrt{\frac{\Delta\rho g d_h}{\rho_L}}$$

u_D is the drift velocity of the gas, describing the buoyancy effect, the effect of local relative velocity between bubbles and liquid.

M. Xu et al. / Catalysis Today 147S (2009) S132–S137

Now as per Xu et al. model, they have actually developed one that relationship between that liquid hold-up with the operating variables. So in that case, for the gas-liquid system, if gas and liquids are flowing at a certain velocity, you can calculate the liquid holdup from this relationship, that

$$\varepsilon_L = 1 - \frac{u_{G,s}}{C_0(u_{G,s}+u_{L,s})+u_D}$$

So from this relationship you can get directly what should be the liquid holdup. Once you know this gas velocity and liquid velocity, of course here one of the important factor is called C_0 here.

This C_0 is called the distribution coefficient which actually describe the effect of velocity and concentration profiles within the mixture of the gas-liquid which is flowing through the channel. And also it accounts for the interaction of the velocity and bubble phase holdup distributions. Another factor is called u_D, this is called drift velocity of the gas which actually describes the bouncy effect and also it is the effect of the local relative velocity between bubbles and liquid. So this C_0 and u_D that actually depends on the you know that fluid properties as well as that geometry of the channel.

Now C_0 that is distribution coefficient is actually mainly depends on the ratio of gas and liquid densities. And you can calculate from this equation.

$$C_0 = 1.2 - 0.2\sqrt{\frac{\rho_G}{\rho_L}}$$

Whereas the drift velocity, it is a function of physical properties of the system like density and also that the geometry of the channels, that is hydraulic diameter. So from this equation,

$$u_D = 0.35\sqrt{\frac{\Delta \rho g d_h}{\rho_L}}$$

you can calculate what should be the u_D. So once you will have this C_0 and u_D you can directly calculate what will be the liquid holdup.

And gas holdup simply you can calculate also by this equation here given.

$$\varepsilon_G = \frac{u_{G,s}}{C_0(u_{G,s} + u_{L,s}) + u_D}$$

So this is simply that ε_G is called gas holdup and ε_L is called liquid holdup. This summation of this liquid hold-up and gas hold-up should be is equal to 1 for gas-liquid system.

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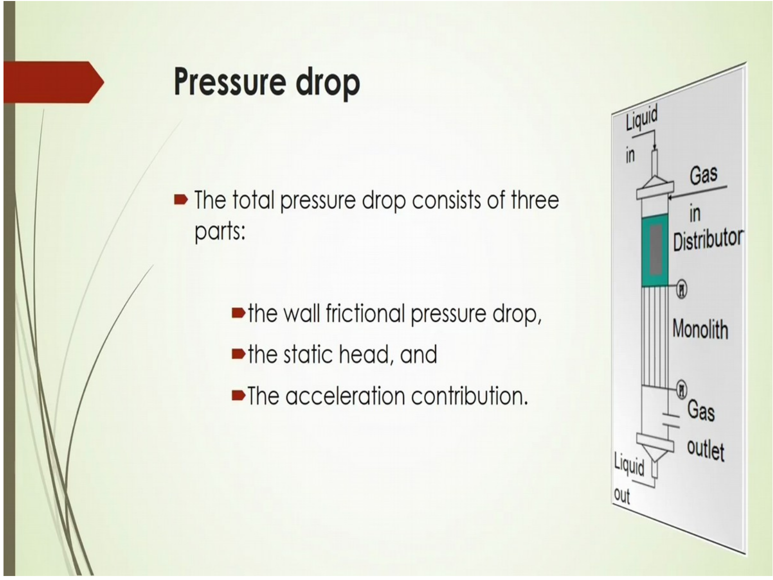

Pressure drop

- The total pressure drop consists of three parts:
  - the wall frictional pressure drop,
  - the static head, and
  - The acceleration contribution.

And another important factor is that pressure drop. Pressure drop is main important factor in that flow resistance to get that different flow regime as well as that mass transfer characteristics there.

So in that case, the wall frictional pressure drop, the static head and acceleration contribution will be there in the total pressure drop.

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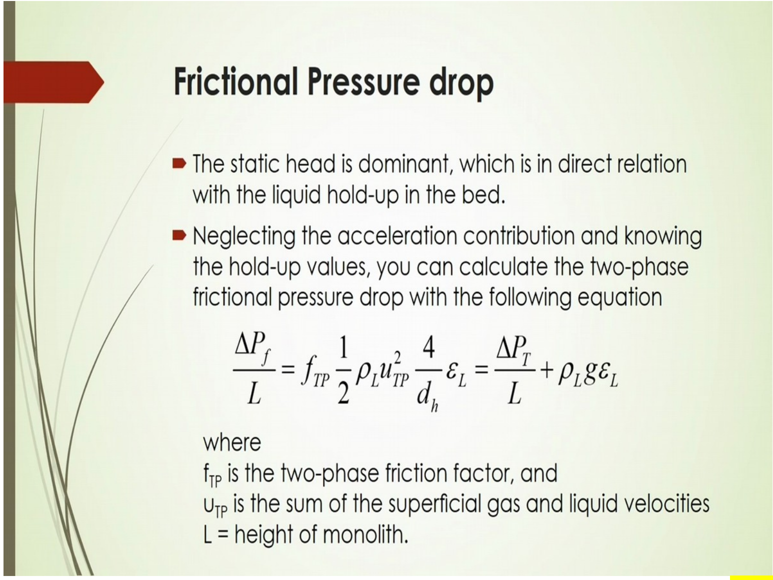

Frictional Pressure drop

- The static head is dominant, which is in direct relation with the liquid hold-up in the bed.
- Neglecting the acceleration contribution and knowing the hold-up values, you can calculate the two-phase frictional pressure drop with the following equation

$$\frac{\Delta P_f}{L} = f_{TP}\frac{1}{2}\rho_L u_{TP}^2 \frac{4}{d_h}\varepsilon_L = \frac{\Delta P_T}{L} + \rho_L g \varepsilon_L$$

where

f_{TP} is the two-phase friction factor, and

u_{TP} is the sum of the superficial gas and liquid velocities

L = height of monolith.

Now the static head is dominant which is in direct relation with the liquid holdup in the bed and neglecting the acceleration contribution and knowing the holdup values you can calculate the two phase frictional pressure drop with the following equation here given.

$$\frac{\Delta P_f}{L} = f_{TP}\frac{1}{2}\rho_L u_{TP}^2 \frac{4}{d_h}\varepsilon_L = \frac{\Delta P_T}{L} + \rho_L g \varepsilon_L$$

Where f_{TP} is the two phase friction factor and u_{TP} is called the sum of the superficial gas and liquid velocities, where L is called the height of the monolith.

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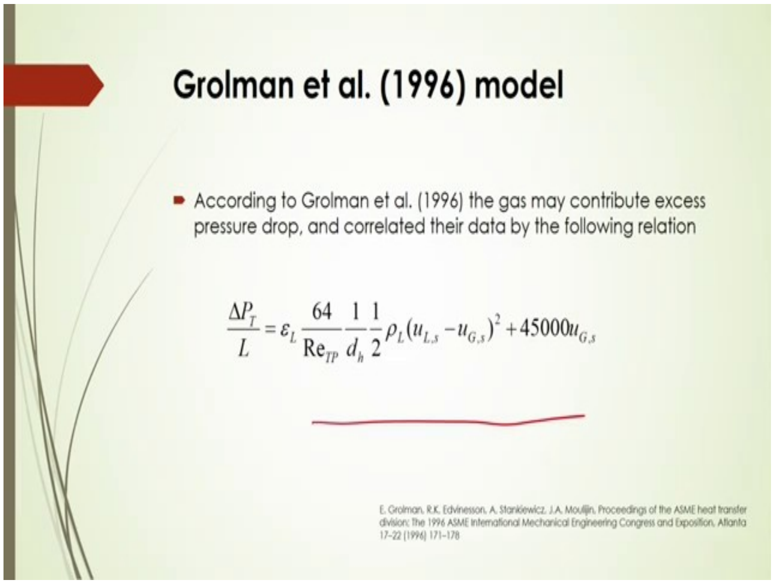

Grolman et al. (1996) model

- According to Grolman et al. (1996) the gas may contribute excess pressure drop, and correlated their data by the following relation

$$\frac{\Delta P_T}{L} = \varepsilon_L \frac{64}{\mathrm{Re}_{TP}} \frac{1}{d_h} \frac{1}{2} \rho_L (u_{L,s} - u_{G,s})^2 + 45000 u_{G,s}$$

E. Grolman, R.K. Edvinesson, A. Stankiewicz, J.A. Moulijn, Proceedings of the ASME heat transfer division: The 1996 ASME International Mechanical Engineering Congress and Exposition, Atlanta 17-22 (1996) 171-178

And according to the Grolman et al. model given in 1996, they have suggested one correlation based on their experimental data to obtain that total frictional pressure drop based on this equation.

$$\frac{\Delta P_T}{L} = \varepsilon_L \frac{64}{\mathrm{Re}_{TP}} \frac{1}{d_h} \frac{1}{2} \rho_L (u_{L,s} - u_{G,s})^2 + 45000 u_{G,s}$$

So you can directly obtain that what should be the fictional pressure drop at your particular operating condition once you know that gas and liquid velocity and your physical properties of the system.

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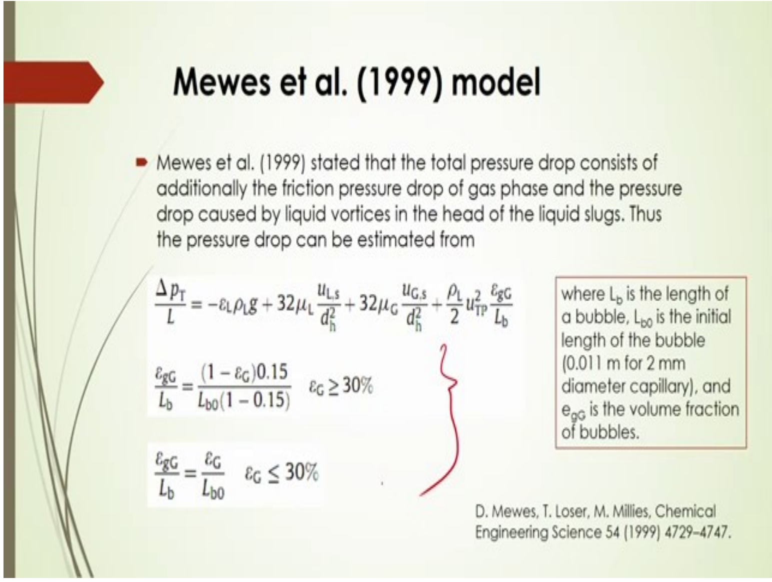

Mewes et al. (1999) model

- Mewes et al. (1999) stated that the total pressure drop consists of additionally the friction pressure drop of gas phase and the pressure drop caused by liquid vortices in the head of the liquid slugs. Thus the pressure drop can be estimated from

$$\frac{\Delta p_T}{L} = -\varepsilon_L \rho_L g + 32\mu_L \frac{u_{L,s}}{d_h^2} + 32\mu_G \frac{u_{G,s}}{d_h^2} + \frac{\rho_L}{2} u_{TP}^2 \frac{\varepsilon_{gG}}{L_b}$$

$$\frac{\varepsilon_{gG}}{L_b} = \frac{(1-\varepsilon_G)0.15}{L_{b0}(1-0.15)} \qquad \varepsilon_G \geq 30\%$$

$$\frac{\varepsilon_{gG}}{L_b} = \frac{\varepsilon_G}{L_{b0}} \qquad \varepsilon_G \leq 30\%$$

where L_b is the length of a bubble, L_{b0} is the initial length of the bubble (0.011 m for 2 mm diameter capillary), and e_{gG} is the volume fraction of bubbles.

D. Mewes, T. Loser, M. Millies, Chemical Engineering Science 54 (1999) 4729–4747.

Similarly other models also can be used like Mewes et al. model here is given in 1999 that this model actually stated that the total pressure drop will be based on that additional frictional pressure drop of gas phase and the pressure drop that is caused by the liquid vortices in the head of the liquid slugs. Thus the pressure drop can be estimated from this equation here.

$$\frac{\Delta P_T}{L} = \varepsilon_L \rho_L g + 32\mu_L \frac{u_{L,s}}{d_h^2} + 32\mu_G \frac{u_{G,s}}{d_h^2} + \frac{0.5\rho_L u_{TP}^2 \varepsilon_{gG}}{L_b}$$

$$\frac{\varepsilon_{gG}}{L_b} = \frac{0.15(1-\varepsilon_G)}{L_{b0}(1-0.15)}; \qquad \varepsilon_G \quad 30\%$$

$$\frac{\varepsilon_{gG}}{L_b} = \frac{\varepsilon_G}{L_{b0}}; \qquad \varepsilon_G \leq 30\%$$

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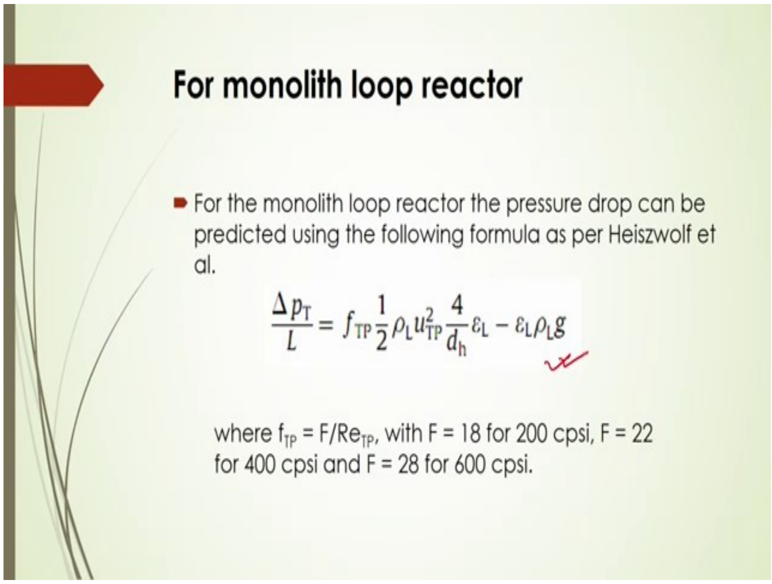

For monolith loop reactor

- For the monolith loop reactor the pressure drop can be predicted using the following formula as per Heiszwolf et al.

$$\frac{\Delta p_T}{L} = f_{TP}\frac{1}{2}\rho_L u_{TP}^2 \frac{4}{d_h}\varepsilon_L - \varepsilon_L \rho_L g$$

where $f_{TP} = F/Re_{TP}$, with F = 18 for 200 cpsi, F = 22 for 400 cpsi and F = 28 for 600 cpsi.

And for monolithic loop reactor, you can say that the pressure drop can be predicted using the following formula as given by that Heiszwolf et al.,

$$\frac{\Delta p_T}{L} = f_{TP}\frac{1}{2}\rho_L u_{TP}^2 \frac{4}{d_h}\varepsilon_L - \rho_L g \varepsilon_L$$

so this also important to calculate that fictional pressure drop here based on this equation.

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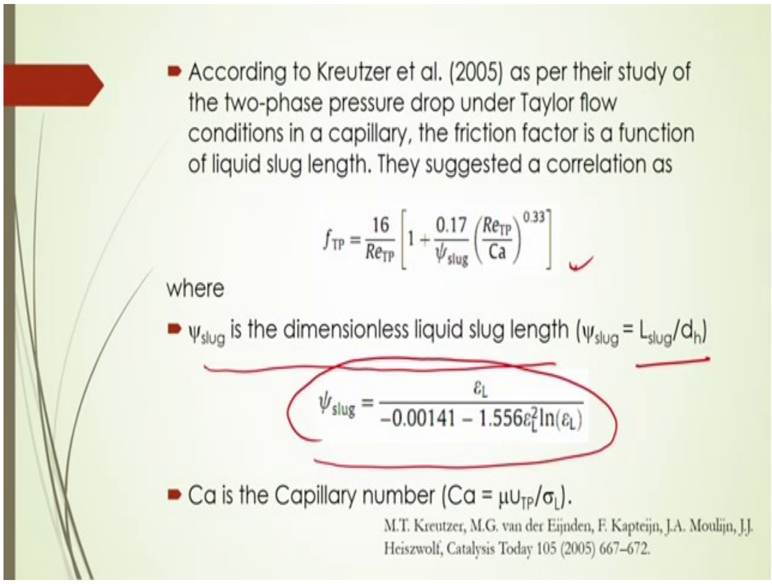

- According to Kreutzer et al. (2005) as per their study of the two-phase pressure drop under Taylor flow conditions in a capillary, the friction factor is a function of liquid slug length. They suggested a correlation as

$$f_{TP} = \frac{16}{Re_{TP}}\left[1 + \frac{0.17}{\psi_{slug}}\left(\frac{Re_{TP}}{Ca}\right)^{0.33}\right]$$

where

- ψ_{slug} is the dimensionless liquid slug length ($\psi_{slug} = L_{slug}/d_h$)

$$\psi_{slug} = \frac{\varepsilon_L}{-0.00141 - 1.556\varepsilon_L^2 \ln(\varepsilon_L)}$$

- Ca is the Capillary number ($Ca = \mu u_{TP}/\sigma_L$).

M.T. Kreutzer, M.G. van der Eijnden, F. Kapteijn, J.A. Moulijn, J.J. Heiszwolf, Catalysis Today 105 (2005) 667–672.

And according to Kreutzer et al. 2005, they have also suggested the two-phase pressure drop under Taylor flow condition in a capillary and in that case the friction factor is a function of liquid slug length and they suggested a correlation like this

$$f_{TP} = \frac{16}{\mathrm{Re}_{TP}}\left[1 + \frac{0.17}{\psi_{slug}}\left(\frac{\mathrm{Re}_{TP}}{Ca}\right)^{0.33}\right]$$

here where ψ_{slug} is the dimensionless liquid slug.

$$\psi_{slug} = \frac{\varepsilon_L}{-0.00141 - 1.556\varepsilon_L^2 \ln(\varepsilon_L)}$$

It is very important to know the, and it will be a function of that L_{slug} and also that slug length and hydraulic diameter. And correlation also they have proposed to calculate that this ψ_{slug} that is ratio of that length of the slugs to the hydraulic diameter.

And based on these calculation, you can obtain what should be the friction factor for that particular monolithic reactor where two phase systems are used for that particular chemical engineering process in the slug flow regime.

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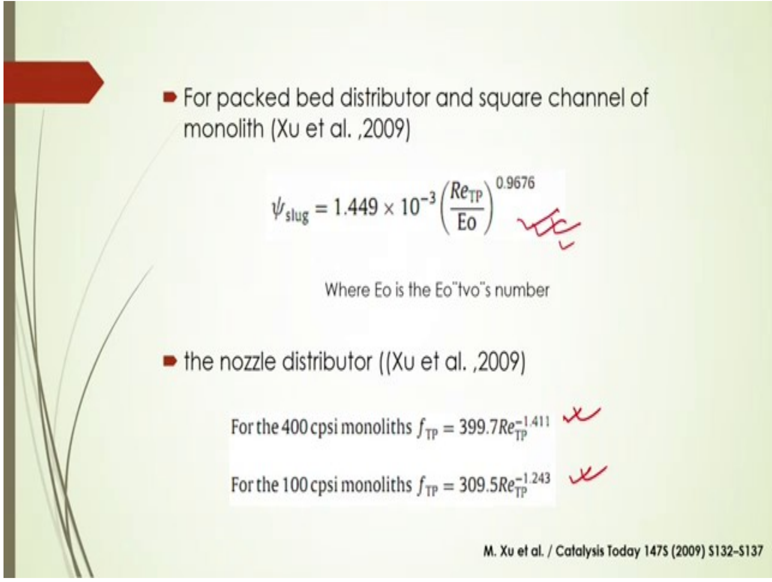

- For packed bed distributor and square channel of monolith (Xu et al. ,2009)

$$\psi_{slug} = 1.449 \times 10^{-3}\left(\frac{Re_{TP}}{Eo}\right)^{0.9676}$$

Where Eo is the Eo¨tvo¨s number

- the nozzle distributor ((Xu et al. ,2009)

For the 400 cpsi monoliths $f_{TP} = 399.7Re_{TP}^{-1.411}$

For the 100 cpsi monoliths $f_{TP} = 309.5Re_{TP}^{-1.243}$

M. Xu et al. / Catalysis Today 147S (2009) S132–S137

And for the packed bed distributor and square channel of monolith Xu et al. also, they have proposed this ψ_{slug} of this ratio of that liquid slugs to the that hydraulic diameter as given in this equation.

$$\psi_{slug} = 1.1449 \times 10^{-3}\left(\frac{\mathrm{Re}_{TP}}{Eo}\right)^{0.9676}$$

The nozzle distributor, if it is used, then the friction factor and for the 400 cpsi and for 100 cpsi, they have proposed these correlations

$$\text{For the 400 cpsi monoliths, } f_{TP} = 399.7\,\mathrm{Re}_{TP}^{-1.411}$$

$$\text{For the 100 cpsi monoliths, } f_{TP} = 309.5\,\mathrm{Re}_{TP}^{-1.243}$$

to calculate that friction factor.

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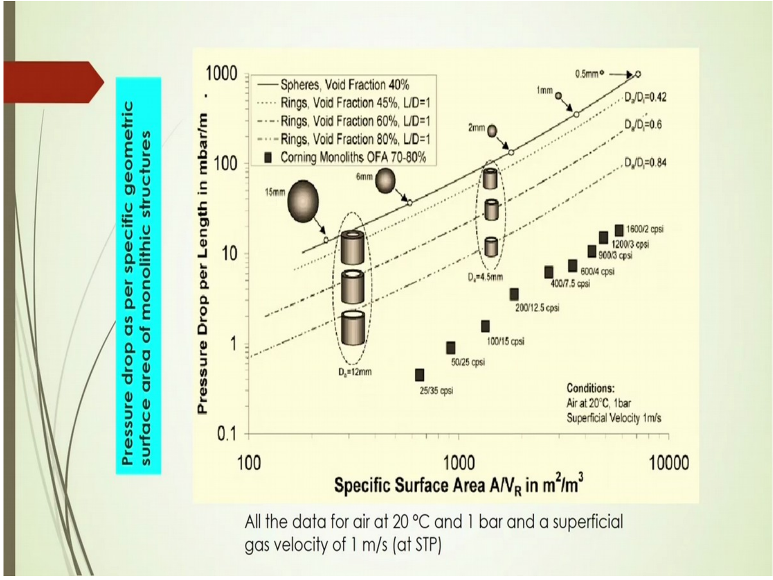

Pressure drop as per specific geometric surface area of monolithic structures

All the data for air at 20 °C and 1 bar and a superficial gas velocity of 1 m/s (at STP)

And in these slides, you can have different that pressure drop per unit length as per specific surface area as per that different surface area how you can get that pressure drop at a different cell density, that you can get from these slides to calculate the pressure drop.

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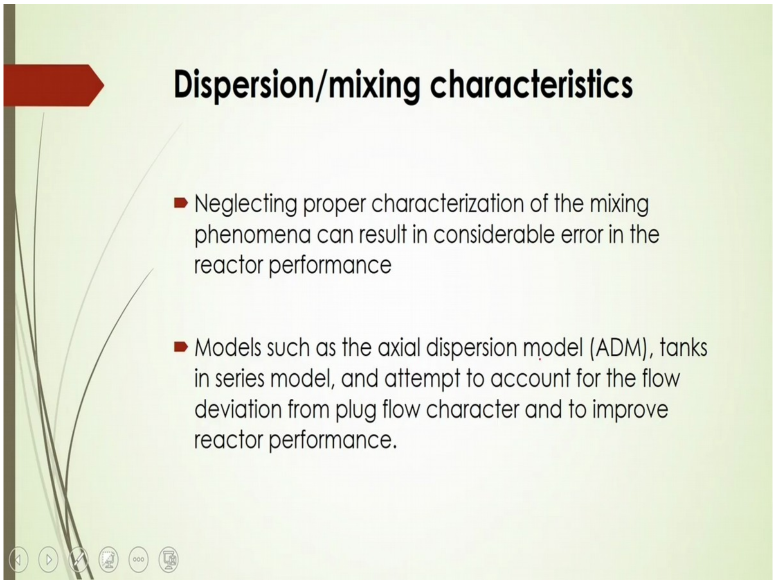

Dispersion/mixing characteristics

- Neglecting proper characterization of the mixing phenomena can result in considerable error in the reactor performance
- Models such as the axial dispersion model (ADM), tanks in series model, and attempt to account for the flow deviation from plug flow character and to improve reactor performance.

And another important factor of this characterizing that monolithic reactor based on that hydrodynamic is called that mixing characteristics. In this case neglecting the proper characterization of the mixing phenomena that can result in considerable error in the reactor performance and in that case, models such as axial dispersion model, tanks in series model and attempt to account for the flow deviation from the plug flow character and to improve reactor performance you have to analyse that mixing characteristic based on that model.

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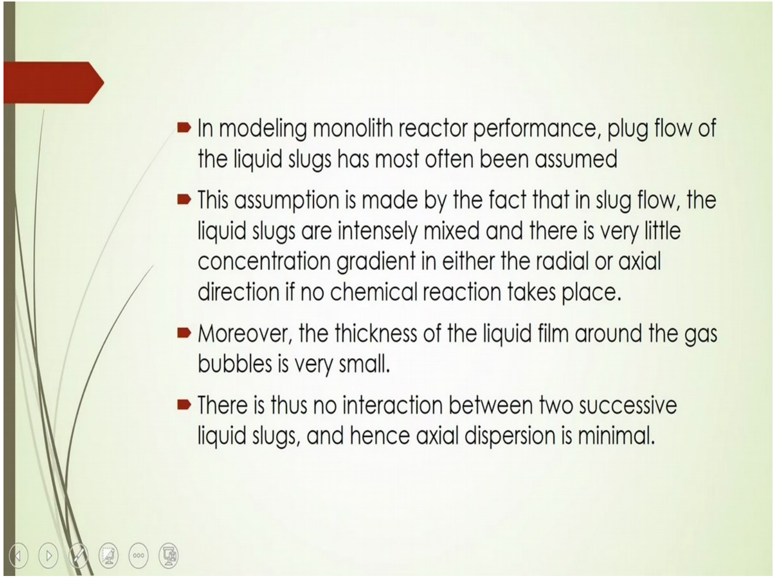

- In modeling monolith reactor performance, plug flow of the liquid slugs has most often been assumed
- This assumption is made by the fact that in slug flow, the liquid slugs are intensely mixed and there is very little concentration gradient in either the radial or axial direction if no chemical reaction takes place.
- Moreover, the thickness of the liquid film around the gas bubbles is very small.
- There is thus no interaction between two successive liquid slugs, and hence axial dispersion is minimal.

And in modeling monolithic reactor performance, plug flow of the liquid slugs has most often been assumed and in that case, the assumption is made by the fact that in the slug flow, the liquid slugs are intensely mixed and there is very little concentration gradient in the either the radial or that axial direction if there is no chemical reaction takes place. Moreover, the thickness of the liquid film around the gas bubbles is very small. So there is thus no interaction between the two successive liquid slugs in the monolithic reactor and hence axial dispersion will be minimal.

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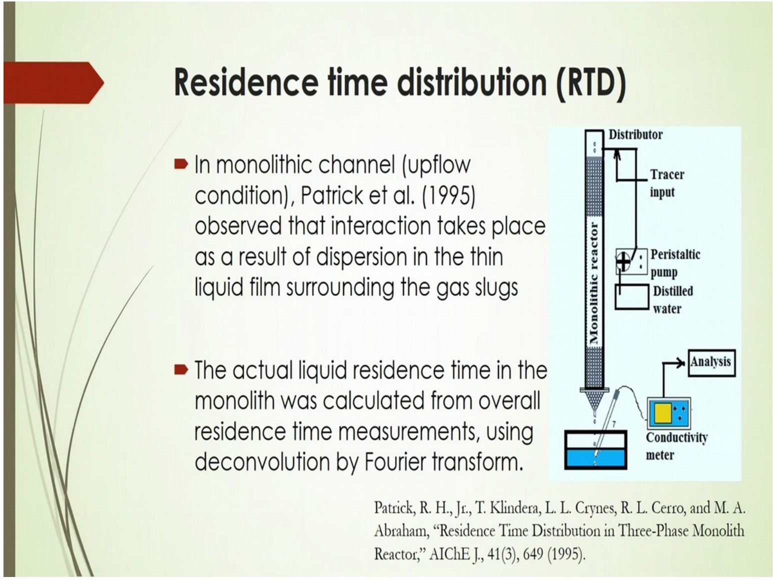

Residence time distribution (RTD)

- In monolithic channel (upflow condition), Patrick et al. (1995) observed that interaction takes place as a result of dispersion in the thin liquid film surrounding the gas slugs
- The actual liquid residence time in the monolith was calculated from overall residence time measurements, using deconvolution by Fourier transform.

Patrick, R. H., Jr., T. Klindera, L. L. Crynes, R. L. Cerro, and M. A. Abraham, "Residence Time Distribution in Three-Phase Monolith Reactor," AIChE J., 41(3), 649 (1995).

And that can be obtained by the residence time distribution method by tracer techniques, just inserting some tracer and collecting the sample and analysing the tracer with respect to time. Then fitting that concentration versus time data with that models.

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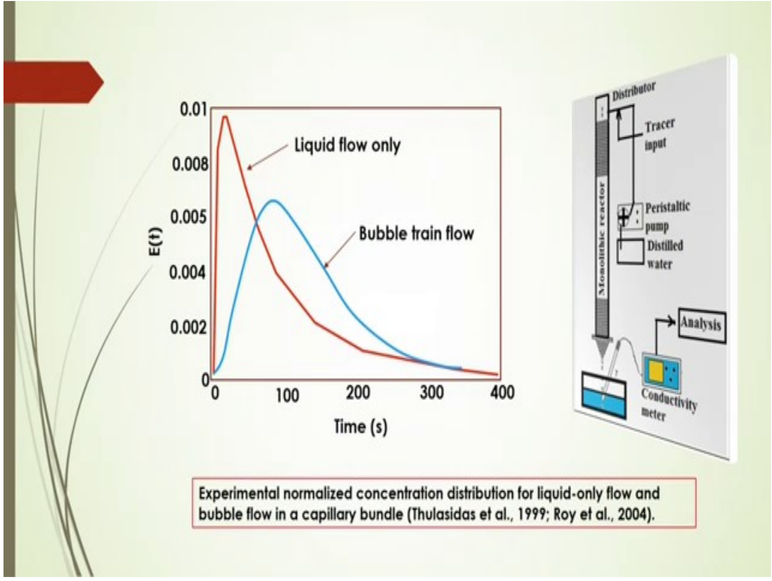
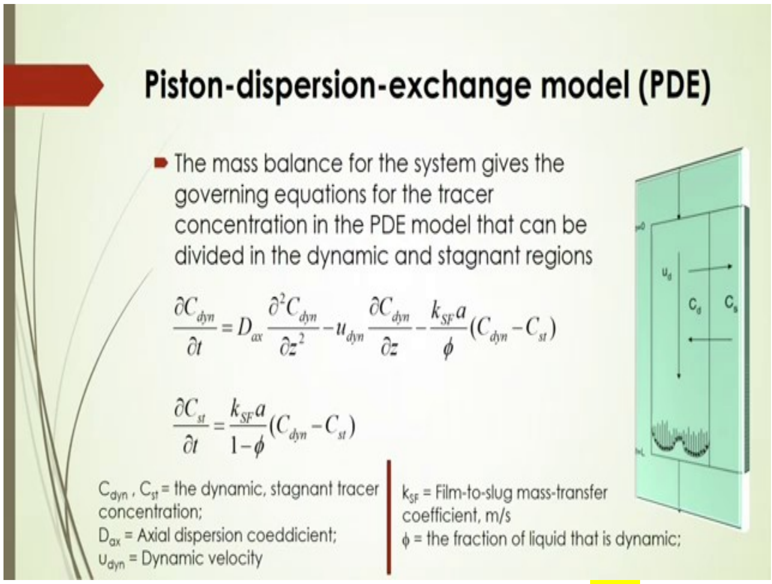


Experimental normalized concentration distribution for liquid-only flow and bubble flow in a capillary bundle (Thulasidas et al., 1999; Roy et al., 2004).



Piston-dispersion-exchange model (PDE)

- The mass balance for the system gives the governing equations for the tracer concentration in the PDE model that can be divided in the dynamic and stagnant regions

$$\frac{\partial C_{dyn}}{\partial t} = D_{ax}\frac{\partial^2 C_{dyn}}{\partial z^2} - u_{dyn}\frac{\partial C_{dyn}}{\partial z} - \frac{k_{SF}a}{\phi}(C_{dyn} - C_{st})$$

$$\frac{\partial C_{st}}{\partial t} = \frac{k_{SF}a}{1-\phi}(C_{dyn} - C_{st})$$

C_{dyn}, C_{st} = the dynamic, stagnant tracer concentration;
D_{ax} = Axial dispersion coeddicient;
u_{dyn} = Dynamic velocity

k_{SF} = Film-to-slug mass-transfer coefficient, m/s
ϕ = the fraction of liquid that is dynamic;

Like that this type of models you have to first draw this, that E(t) that is concentration versus time data where you can calculate those that parameter for the mixing characteristics and that axial dispersion coefficient just by fitting this model of this Piston-dispersion-exchange model.

$$\frac{\partial C_{dyn}}{\partial t} = D_{ax}\frac{\partial^2 C_{dyn}}{\partial z^2} - u_{dyn}\frac{\partial C_{dyn}}{\partial z} - \frac{k_{SF}a}{\phi}(C_{dyn} - C_{st})$$

$$\frac{\partial C_{st}}{\partial t} = \frac{k_{SF}a}{1-\phi}(C_{dyn} - C_{st})$$

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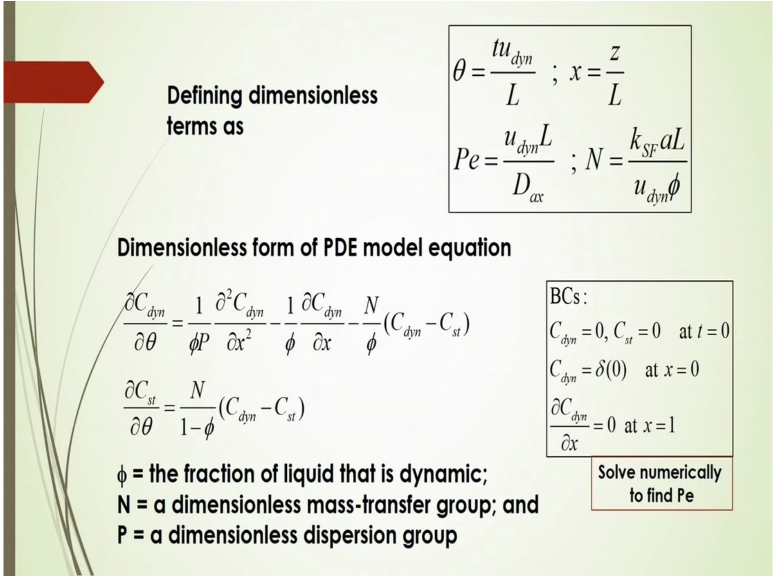


Defining dimensionless terms as

$$\theta = \frac{tu_{dyn}}{L} \; ; \; x = \frac{z}{L}$$

$$Pe = \frac{u_{dyn}L}{D_{ax}} \; ; \; N = \frac{k_{SF}aL}{u_{dyn}\phi}$$

Dimensionless form of PDE model equation

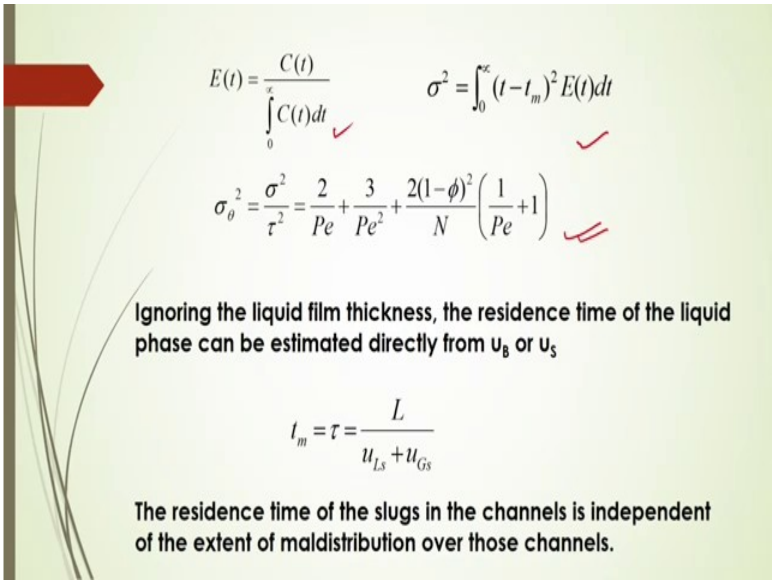
$$\frac{\partial C_{dyn}}{\partial \theta} = \frac{1}{\phi P}\frac{\partial^2 C_{dyn}}{\partial x^2} - \frac{1}{\phi}\frac{\partial C_{dyn}}{\partial x} - \frac{N}{\phi}(C_{dyn} - C_{st})$$

$$\frac{\partial C_{st}}{\partial \theta} = \frac{N}{1-\phi}(C_{dyn} - C_{st})$$

BCs:
$C_{dyn} = 0, C_{st} = 0 \quad \text{at } t = 0$
$C_{dyn} = \delta(0) \quad \text{at } x = 0$
$\frac{\partial C_{dyn}}{\partial x} = 0 \quad \text{at } x = 1$

Solve numerically to find Pe

ϕ = the fraction of liquid that is dynamic;
N = a dimensionless mass-transfer group; and
P = a dimensionless dispersion group



$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} \checkmark \qquad \sigma^2 = \int_0^\infty (t - t_m)^2 E(t) dt \checkmark$$

$$\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \frac{2}{Pe} + \frac{3}{Pe^2} + \frac{2(1-\phi)^2}{N}\left(\frac{1}{Pe} + 1\right) \checkmark\checkmark$$

Ignoring the liquid film thickness, the residence time of the liquid phase can be estimated directly from u_B or u_S

$$t_m = \tau = \frac{L}{u_{Ls} + u_{Gs}}$$

The residence time of the slugs in the channels is independent of the extent of maldistribution over those channels.

And according to this model, you will get the different parameters like that it is defined as per a given information in the slides.

$$\frac{\partial C_{dyn}}{\partial \theta} = \frac{1}{\phi P}\frac{\partial^2 C_{dyn}}{\partial x^2} - \frac{1}{\phi}\frac{\partial C_{dyn}}{\partial x} - \frac{N}{\phi}(C_{dyn} - C_{st})$$

$$\frac{\partial C_{st}}{\partial \theta} = \frac{N}{1-\phi}(C_{dyn} - C_{st})$$

$$\theta = \frac{t u_{dyn}}{L} \;\; ; \;\; x = \frac{z}{L}$$

$$Pe = \frac{u_{dyn} L}{D_{ax}} \;\; ; \; N = \frac{k_{SF} a L}{u_{dyn} \phi}$$

BCs :

$C_{dyn} = 0,\ C_{st} = 0 \quad \text{at } t = 0$

$C_{dyn} = \delta(0) \quad \text{at } x = 0$

$\frac{\partial C_{dyn}}{\partial x} = 0 \ \text{ at } x = 1$

Some that fraction of the liquid that is dynamic, even some dimensionless parameters, here mass transfer group and also Peclet number here, dispersion groups here that is defined in the slides here. So based on this model, you have to first calculate that what will be the E(t). E(t), it would be calculated by here,

$$E(t) = C(t) / \int_0^{\infty} C(t)dt$$

it is given here and then from that model you have to calculate that, that by moment method what would be the σ^2, that is called the variance of that model.

$$\sigma^2 = \int_0^{\infty} (t - t_m)^2 E(t)dt$$

And once you know that variance, you can correlate this variance with this Peclet number as,

$$\sigma_\theta{}^2 = \frac{\sigma^2}{\tau^2} = \frac{2}{Pe} + \frac{3}{Pe^2} + \frac{2(1-\phi)^2}{N}\left(\frac{1}{Pe} + 1\right)$$

That Peclet number will give you that intensity of the mixing, that is 1 by Peclet number it is called the dispersion number. If you are getting more dispersion number, you may get that more intensity of the mixing inside the reactor and also degree of mixing you can say. That based on that degree of mixing you can say what should be the that average residence time of the liquid phase in the reactor

$$t_m = \tau = \frac{L}{u_{Ls} + u_{Gs}}$$

and which actually directly related to the reaction performance and of the chemical engineering process.

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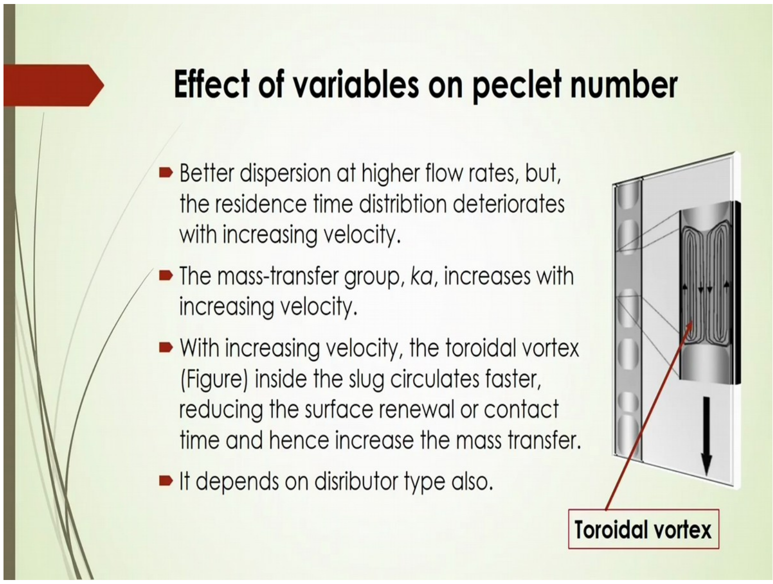

Effect of variables on peclet number

- Better dispersion at higher flow rates, but, the residence time distribtion deteriorates with increasing velocity.
- The mass-transfer group, *ka*, increases with increasing velocity.
- With increasing velocity, the toroidal vortex (Figure) inside the slug circulates faster, reducing the surface renewal or contact time and hence increase the mass transfer.
- It depends on disributor type also.

And also you can say that performance of the reactor based on that mixing characteristics. So how we can get the intensification of that particular process in the monolithic reactor, you can assess it by this mixing processes. So you can say that these mixing processes will be actually depending on that several factors like geometry of the reactor as well as that other operating variables like that physical properties of the system and also operating variables like flow rate of the phases. Also another important the distributor type is one of the important factor because you know that several distributor will give you that different degree of maldistribution of that you know liquid inside the reactor which we may affect that energy distribution in the reactor, how that liquid will be distributed inside the reactor based on that energy dissipation.

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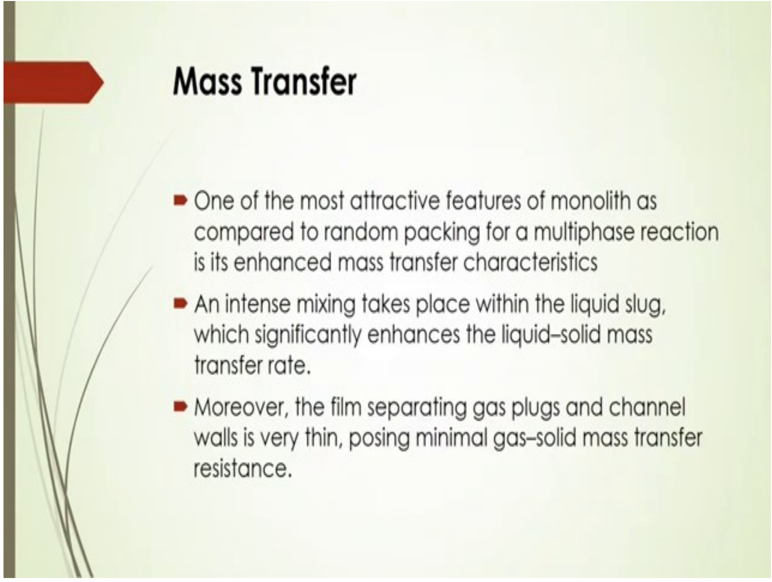
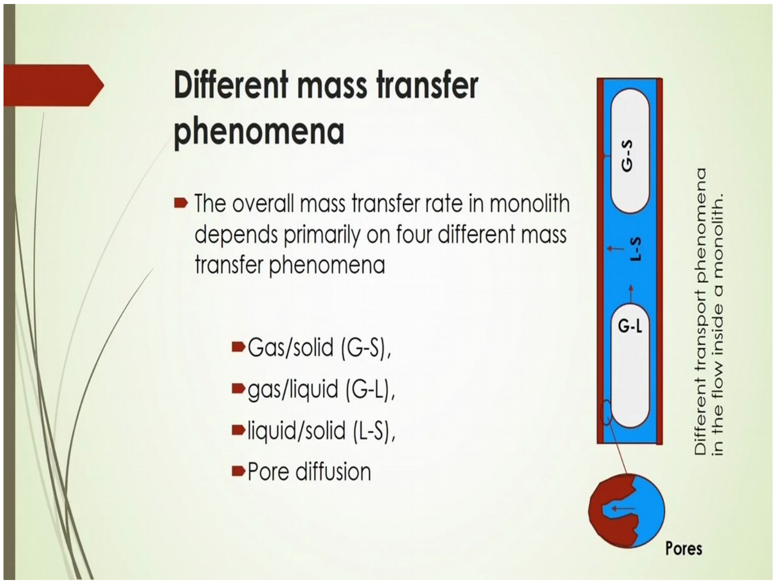


Mass Transfer

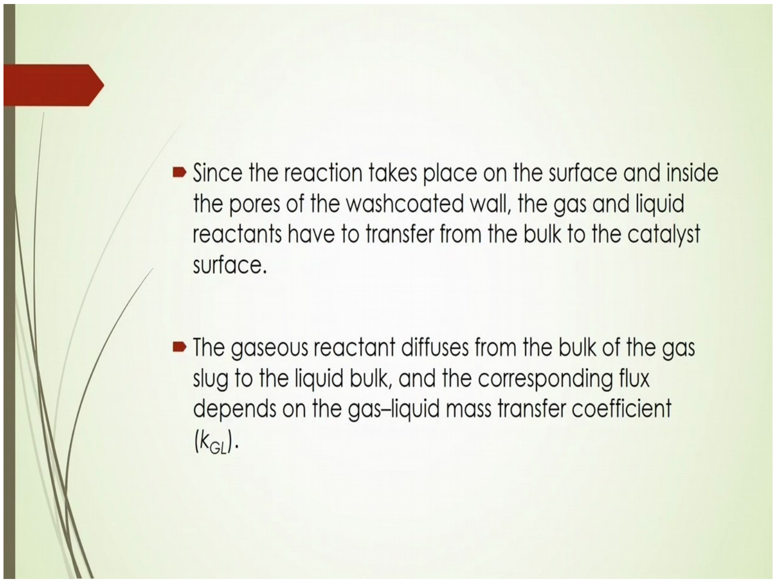
- One of the most attractive features of monolith as compared to random packing for a multiphase reaction is its enhanced mass transfer characteristics
- An intense mixing takes place within the liquid slug, which significantly enhances the liquid–solid mass transfer rate.
- Moreover, the film separating gas plugs and channel walls is very thin, posing minimal gas–solid mass transfer resistance.



Different mass transfer phenomena

- The overall mass transfer rate in monolith depends primarily on four different mass transfer phenomena
  - Gas/solid (G-S),
  - gas/liquid (G-L),
  - liquid/solid (L-S),
  - Pore diffusion

Different transport phenomena in the flow inside a monolith.



- Since the reaction takes place on the surface and inside the pores of the washcoated wall, the gas and liquid reactants have to transfer from the bulk to the catalyst surface.
- The gaseous reactant diffuses from the bulk of the gas slug to the liquid bulk, and the corresponding flux depends on the gas–liquid mass transfer coefficient (k_{GL}).

Now again that mixing characteristic affect that mass transfer phenomena and different mass transfer phenomena like gas liquid, gas liquid solid, liquid solid and pore distribution here as per slides given. And also different types of mass transfer coefficients based on that gas liquid solid, liquid solid like these.

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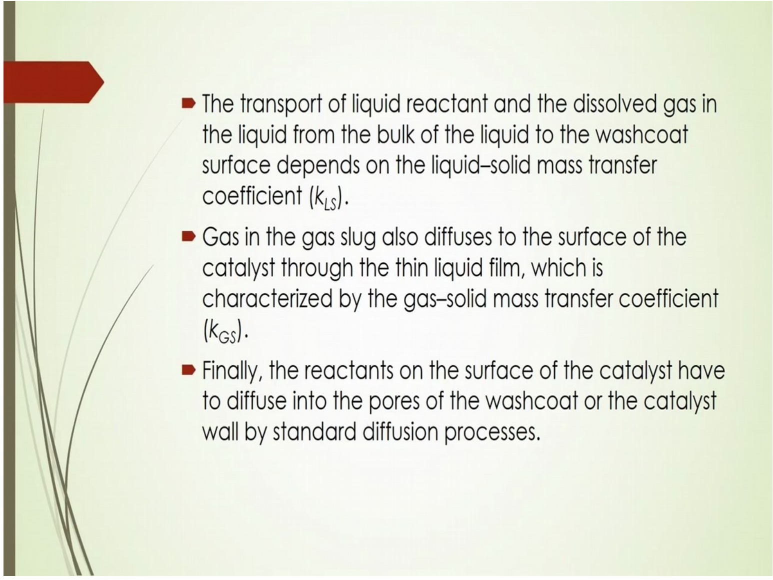
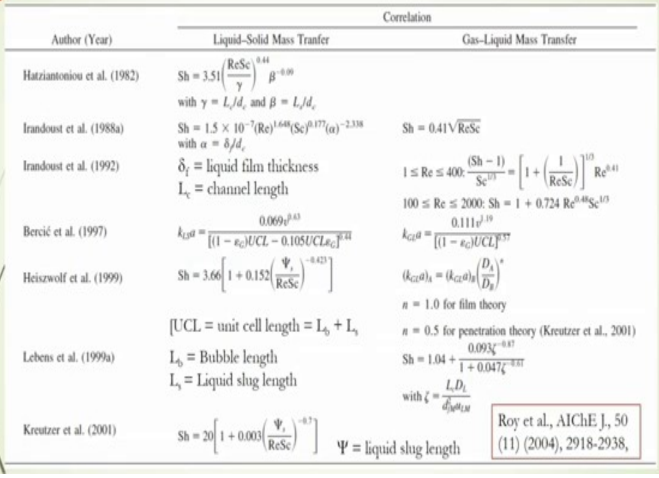


- The transport of liquid reactant and the dissolved gas in the liquid from the bulk of the liquid to the washcoat surface depends on the liquid–solid mass transfer coefficient (k_{LS}).
- Gas in the gas slug also diffuses to the surface of the catalyst through the thin liquid film, which is characterized by the gas–solid mass transfer coefficient (k_{GS}).
- Finally, the reactants on the surface of the catalyst have to diffuse into the pores of the washcoat or the catalyst wall by standard diffusion processes.



Author (Year)	Correlation Liquid–Solid Mass Tranfer	 Gas–Liquid Mass Transfer
Hatziantoniou et al. (1982)	$Sh = 3.51\left(\frac{ReSc}{\gamma}\right)^{0.44}\beta^{-0.09}$ with $\gamma = L_c/d_c$ and $\beta = L_s/d_c$	
Irandoust et al. (1988a)	$Sh = 1.5 \times 10^{-7}(Re)^{1.648}(Sc)^{0.177}(\alpha)^{-2.338}$ with $\alpha = \delta_f/d_c$	$Sh = 0.41\sqrt{ReSc}$
Irandoust et al. (1992)	δ_f = liquid film thickness L_c = channel length	$1 \le Re \le 400: \frac{(Sh-1)}{Sc^{1/3}} = \left[1 + \left(\frac{1}{ReSc}\right)\right]^{1/3} Re^{0.41}$ $100 \le Re \le 2000: Sh = 1 + 0.724\, Re^{0.48} Sc^{1/3}$
Berčić et al. (1997)	$k_{LS}a = \frac{0.069v^{0.63}}{[(1-\varepsilon_G)UCL - 0.105UCL\varepsilon_G]^{0.44}}$	$k_{GL}a = \frac{0.111v^{1.19}}{[(1-\varepsilon_G)UCL]^{0.57}}$
Heiszwolf et al. (1999)	$Sh = 3.66\left[1 + 0.152\left(\frac{\Psi_s}{ReSc}\right)^{-0.423}\right]$	$(k_{GL}a)_A = (k_{GL}a)_B\left(\frac{D_A}{D_B}\right)^n$ $n = 1.0$ for film theory
	[UCL = unit cell length = $L_b + L_s$	$n = 0.5$ for penetration theory (Kreutzer et al., 2001)
Lebens et al. (1999a)	L_b = Bubble length L_s = Liquid slug length	$Sh = 1.04 + \frac{0.093\zeta^{-0.87}}{1 + 0.047\zeta^{-0.61}}$ with $\zeta = \frac{L_sD_L}{d_{ch}^2 u_{LM}}$
Kreutzer et al. (2001)	$Sh = 20\left[1 + 0.003\left(\frac{\Psi_s}{ReSc}\right)^{-0.7}\right]$	Ψ = liquid slug length

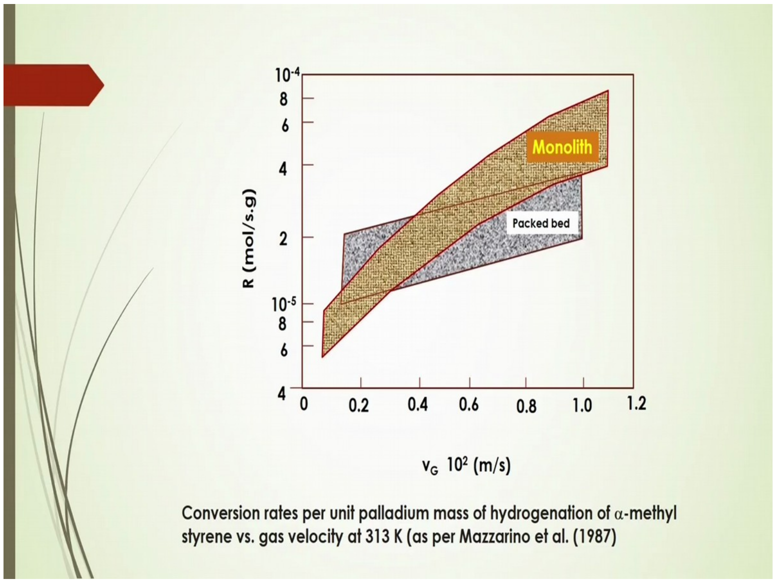
Roy et al., AIChE J., 50 (11) (2004), 2918-2938,

Gas–solid mass transfer

- The gaseous reactant diffuses to the solid surface through the thin film surrounding the gas slug.
- The thin-film model can therefore be used to determine the gas–solid mass transfer coefficient

$$k_{G-S} = \frac{D}{\delta_f}$$

- Therefore, to determine the gas–solid mass transfer coefficient, one has to evaluate the film thickness (δ_f) of the liquid film, which depends primarily on the surface tension of the liquid and the liquid diffusivity (*D*).



Conversion rates per unit palladium mass of hydrogenation of α-methyl styrene vs. gas velocity at 313 K (as per Mazzarino et al. (1987)

So here, these are the slides that you can go through in more details to get that you know even for mass transfer coefficient calculation from the correlation

$$k_{G-S} = \frac{D}{\delta_f}$$

and what are the effects and how that has solid mass transfer happens and what are the different regimes of that reaction, rates based on that mass transfer coefficient and also that comparison of the monolithic and packed bed reactors there.

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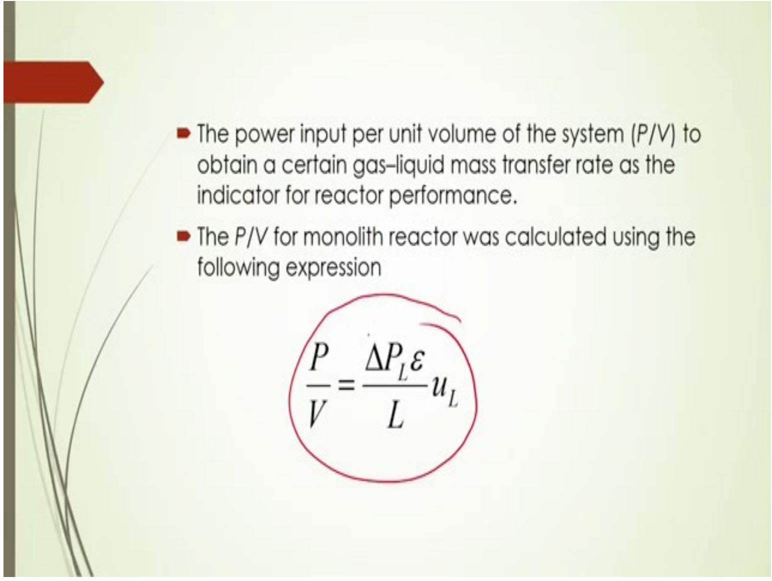

- The power input per unit volume of the system (*P*/*V*) to obtain a certain gas–liquid mass transfer rate as the indicator for reactor performance.
- The *P*/*V* for monolith reactor was calculated using the following expression

$$\frac{P}{V} = \frac{\Delta P_L \varepsilon}{L} u_L$$

So and also how that energy is being actually distributed and how to calculate that energy or power into per unit volume of the system to calculate that mixing characteristics and also the mass transfer characteristics.

$$\frac{P}{V} = \frac{\Delta P_L \varepsilon}{L} u_L$$

So that power can be calculated based on this equation. So once you know that energy distribution and what will be that efficiency of the reactor you can calculate. So I would like to stop here, this module of this you know that monolithic structure and its use and application and also different hydrodynamic aspects and we will start the next lecture onward, another module for the process intensification.

(Refer Slide Time: 59:59)

Further reading......

- Kamelia Boodhoo and Adam Harvey. Process Intensification for Green Chemistry Engineering Solutions for Sustainable Chemical Processing, Edited by Kamelia Boodhoo and Adam Harvey , School of Chemical Engineering & Advanced Materials Newcastle University, UK. Willey, 2013
- Juan Gabriel Segovia-Hernández, Adrián Bonilla-Petriciolet Editors, Process Intensication in Chemical Engineering Design Optimization and Control, Springer, 2016.
- David Reay, Colin Ramshaw, and Adam Harvey, Process Intensification: Engineering for effgiciency, sustainability and flexibility, IchemE, 2nd edition, 2013, Elsevier.

I would suggest you to go further reading for this monolithic structure and its application and also different hydrodynamic aspects. These are the some references that will be helpful for you. So thank you.