

Continuum Mechanics And Transport Phenomena
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Lecture – 02
Measurement and Prediction - Part 2

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Scope of transport phenomena

- Predict actual performance / size of the equipment
 - Power required for compression of the feed gas – **Minimum Actual value**
 - Conversion of hydrogen in the reactor – **Maximum Actual value**
 - Composition of vapour leaving the condenser/refrigerator – **Equilibrium value Actual value**
 - Size of reactor (Mass of catalyst required - Length of tubes, number of tubes)
 - Size of condenser/refrigerator (Heat exchanger area - Length of tubes, number of tubes)
 - Size of liquid vapour separator (Height, diameter)

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Now, how does this improve the scope of transport phenomena compared to the scope of thermodynamics? Now, as we predict the actual performance or size of the equipment, what does it mean?. Let us go back to our examples, in the earlier case we predicted the power required for compression of the feed gas, it is a minimum value.

If we predict based on the process calculation course it is less accurate, if you predict based on the thermodynamic course it is still more accurate, but still, it is a minimum value. You are not getting the actual value. But, using a transport phenomena approach you to find out the actual value which will be much more closer to reality.

Now, similarly the conversion of hydrogen in the reactor, we found out the maximum value either based on the assumption that gases behave ideally or they behave non ideally, but still gives the maximum value only. But, using a transport phenomena approach you can find out the actual value of a conversion based on the size of the reactor. And, the composition of

vapour leaving the condenser and refrigerator they were found out assuming phase equilibrium.



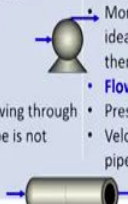
Once again, of lower accuracy with process calculation knowledge still more accuracy with using a thermodynamics knowledge, but still they are equilibrium values. Suppose you want to find out the actual value which is related to the size equipment size heat exchanger then you need to use a transport phenomena approach. So, we have said that the size of the equipment is not under the purview of thermodynamics. The moment we use a transport phenomena approach we can determine the size of the reactor meaning the mass of catalyst, length of tubes, number of tubes.

We can find out the size of the condenser, refrigerator which is a heat exchanger, find out the area of the heat exchanger, the length of tubes, number of tubes, and of course, the size of the liquid vapour separator namely height and diameter. So, to find out the size of these equipment, we need transport phenomena approach and to consider the include the size of these equipment on the performance we require a transport phenomena approach.

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Flow of fluids/Fluid Mechanics/Momentum transfer

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none">• Power required for pumping• Minimum power required for pumping water from one level to another• Neglecting frictional losses	<ul style="list-style-type: none">• Power required for pumping• Calculate the actual power required• Including frictional losses• More work to be supplied than the ideal work predicted from thermodynamics
<ul style="list-style-type: none">• Flow through pipe• Pressure drop for water flowing through constant area horizontal pipe is not considered	<ul style="list-style-type: none">• Flow through pipe• Pressure drop due to friction with wall• Velocity profile across the radius of the pipe



Now, we will take several examples, not necessarily connected to this flow sheet. Take several examples from fluid mechanics, heat transfer, and mass transfer and then compare the scope of thermodynamics and scope of transport phenomena approach. That will also give you what are the scope of transport phenomena and how does it compare with the thermodynamic approach.

So, the first example which are going to consider is the power required for pumping, supposed if we have water to be pumped from one level to another and then we are using a pump. Let us say a household example of pumping water from a sump to an overhead tank. And, if you use a thermodynamic approach that will give you the minimum power required to pump water from one level to another level because it neglects frictional losses, it gives you only the minimum pumping power required.

But, if you use a transport phenomena approach, you can calculate the actual power required. Why is it possible? Because, we include frictional losses, the liquid flows through the pipe losses due to friction happen because of the contact to the wall. We include that so, we can calculate what is the actual work required, the power required to pump water from one level to the other. And so, we know more work has to be supplied compared to the ideal work that is predicted from thermodynamics.




So, the thermodynamic approach gives a minimum work required, transport phenomena approach gives us the actual work required including the friction losses. An analogous example is flow through a pipe; suppose if you have a flow of let us say a liquid flowing through a horizontal pipe with no change in cross-section. The thermodynamic approach will not give us any pressure drop at all. But, if you consider the transport phenomena approach, you include the frictional losses and you can find out the pressure drop due to flow through this pipe, because of friction of the wall.

Also, we can calculate what is the velocity profile across the cross-section of the pipe. The velocity is 0 near the wall and it is maximum at the center of the pipe. So, velocity varies across this cross-section. So, the transport phenomena approach will also help us to find out what is the velocity profile across this pipe. So, one is the transport phenomena approach gives the max; the actual work required. Now, also includes friction and gives the velocity profile as well.

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Flow of energy/heat - Heat transfer (Conduction and convection)

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none">• Furnace wall• Direction of heat transfer• Direction of temperature decrease• Does not consider rate of heat transfer	<ul style="list-style-type: none">• Furnace wall• Considers rate of heat transfer by conduction due to temperature gradient• Calculate<ul style="list-style-type: none">• Rate of heat transfer• Temperature profile
<ul style="list-style-type: none">• Cooling of glass of water• Only final equilibrium temperature• Not how the temperature reaches the equilibrium temperature• Not how long	<ul style="list-style-type: none">• Cooling of glass of water• How the temperature reaches the equilibrium value• How long to reach equilibrium



The next example is from heat transfer; consider two examples here. The first example is heat transfer in a furnace wall, let us say we have a furnace and this is a furnace wall. And, let us say we have a high temperature at the left side of the wall and the low temperature at the right side of the wall. So, what is the scope of thermodynamics? Thermodynamics will tell you the direction of heat transfer and then which is the direction of temperature decrease, but, does not consider the rate of heat transfer.

But, if you use a transport phenomena approach it considers the rate of heat transfer by conduction which is due to the temperature gradient. And, you can calculate what is the rate of heat transfer taking place through this furnace wall and also calculate what is the temperature profile across the width of this furnace wall. Well, thermodynamics tells you the direction of heat transfer, transport phenomena tells you the rate of heat transfer, how fast it takes place. Also, tells you the temperature profile, how temperature varies along with the thickness of the furnace wall.

Now, another simple example would be, suppose if you take little warm water and then place it in an ambient temperature and allow it to cool. What does thermodynamics tell you? It tells you the final equilibrium temperature which is the same as ambient temperature. But, thermodynamics does not tell you how fast the equilibrium will be reached, does not tell you how the temperature varies is a function of time, how long it takes to reach equilibrium.

Now, or how the temperature reaches equilibrium value either linearly, exponentially does not come up from thermodynamic analysis. From the transport phenomena approach, you can find out how the temperature cools down. How the temperatures cool down from the high temperature to the ambient temperature and also find out how long it takes to reach the equilibrium value. So, as we have discussed earlier all the time factor, length factor, area factor are all considered in the transport phenomena approach.

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Flow of energy/heat - Heat transfer (Heat exchanger)

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none"> • Heat exchanger • Given inlet temperatures of hot and cold fluid and one outlet temperature (e.g. hot fluid) • Calculate outlet temperature of cold fluid • Rate of heat transfer is not considered • Does not consider <ul style="list-style-type: none"> • Area/size/length of heat transfer • Direction of flow 	<ul style="list-style-type: none"> • Heat exchanger • Given inlet temperatures of hot and cold fluid and one outlet temperature (e.g. hot fluid) • Rate of heat transfer is considered • Rate of heat transfer proportional to temperature difference • Determine <ul style="list-style-type: none"> • Area/length of heat exchanger • Temperature profile along the length • Is cocurrent or countercurrent better?

Now, another example from heat transfer with respect to the heat exchanger. Let us say the heat exchanger and then you are given two inlet temperatures and then you are given one outlet temperature. And, let us say inlet temperature is the hot and cold fluid, and you are given the outlet temperature of the hot fluid also. Now, using a simple energy balance which is based on thermodynamics you can find out what is the outlet temperature of the fluid and outlet temperature of the cold fluid.

Now, the rate of heat transfer is not considered. So, the area of the heat exchanger which you said is equivalent to size, length etcetera the heat exchanger is not considered. We also do not consider and take into account the direction of the flow whether they flow counter-current to each other or co-current to each other. So, thermodynamics will tell you what is the outlet temperature of cold fluid no doubt about it but does not consider the rate of heat transfer. Hence, the size of the heat exchanger is not considered and does not consider and take into

account what is the influence of the direction of the relative direction of motion between the two streams whether co-current or counter-current.



But, if you use a transport phenomena approach, let us take the same case you have given two inlet temperatures and one outlet temperature. Transport phenomenon approach considers the rate of heat transfer and that rate of heat transfer is proportional to the temperature difference between these two fluid streams, the hot and cold fluid streams. And, hence you can determine the area and length of heat exchanger, what is the temperature profile along the length of the heat exchanger. You can also answer the question whether the counter current mode or a co-current mode is better for contact.

So, just because it takes into account the rate of heat transfer, your scope of analysis, scope of prediction widens a lot. As you have seen here the length of heat exchanger, the temperature profile along the length, and also the influence of relative contacting direction was also taken into account.

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Flow of species - Mass transfer (Diffusion)

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none">• Vapourization of solvent• Raoult's law• Saturation concentration of solvent vapour in the gas at liquid surface• Rate of mass transfer is not considered• Does not give rate of loss of solvent	<ul style="list-style-type: none">• Vapourization of solvent• Considers the rate of mass transfer due to diffusion of solvent vapour• Rate of mass transfer depends on concentration gradient• Determine<ul style="list-style-type: none">• Rate of loss of solvent• Concentration profile of solvent vapour
<ul style="list-style-type: none">• Raw gulab jamoon in sugar syrup• Equilibrium sugar concentration	<ul style="list-style-type: none">• Raw gulab jamoon in sugar syrup• How long it takes for saturation• Concentration profile of sugar inside the jamoon



Now, few examples from a mass transfer. The first example is the vapourization of a solvent. Let us say we have a very volatile solvent and we like to predict the rate of vapourization of the solvent. So, if you use a thermodynamic approach, use Raoult's law. What can Raoult's law give us? Raoult's law can give us what is the concentration of this volatile solvent in the gas which is in just contact with the liquid phase. So, that gives the saturation value and that is the scope of thermodynamics.

And, it does not consider the rate of mass transfer, it does not give the rate of mass loss of solvent. But, if you use the transport phenomena approach, we consider the rate of mass transfer which is your diffusion which is depends on the concentration gradient between let us say the surface of the liquid and the top of the tube. Because, of this we can determine the rate of loss of solvent and the concentration profile along the length of the tube as well.




So, transport phenomena approach considers the rate of mass transfer, in this case is because of diffusion. Diffusion is because of concentration gradient because, of that we can find out or predict what is the rate of loss of solvent. What does it mean? Suppose, if you leave this tube for let us say a day or two how much would the solvent would have been evaporated. And of course, going to be very less quantity, but still you can find out what is the rate of loss of solvent. And of course, you can find out what is the concentration profile of solvent vapour along the length of the tube.

Another household and then mouth-watering example would be let us say have raw gulab jamoon and then putting in sugar syrup, equilibrium sugar concentration can be predicted from thermodynamics. But, if you are very eager to take the gulab jamoon, the transport phenomenon will tell you how long you have to wait. And, still more interested you can predict the concentration profile of sugar inside the gulab jamoon. So, that is the scope of transport phenomena, in terms of rate and then the concentration profile.

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Flow of species - Mass transfer (Absorption)

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none"> Absorption of NH_3 in water in a packed column Henry's law What is the equilibrium concentration of the gas and liquid phases at given T and P – maximum value possible for infinite contact time Rate of mass transfer is not considered Does not consider the height of column, direction of flow 	<ul style="list-style-type: none"> Absorption of NH_3 in water in a packed column Considers rate of mass transfer Rate of mass transfer depends on the difference between equilibrium and actual concentration Determine <ul style="list-style-type: none"> Height of column to achieve a desired % removal e.g. 90 % Axial concentration profile of NH_3 in gas and liquid phase Is cocurrent or countercurrent contact better?

Another example from mass transfer model with chemical engineering application of absorption. Suppose, if you have a stream of air and ammonia and you want to observe ammonia using water, for the thermodynamic approach we use Henry's law. And, then based on that you will find out what is equilibrium concentration of the gas and liquid phases. You are given the let us say the inlet concentration of liquid, you are given the inlet concentration of gas. And, based on Henry's law, based on mass balance you can find out what is the equilibrium concentration of streams leaving; that is a concentration which they were given infinite time and they would attain.

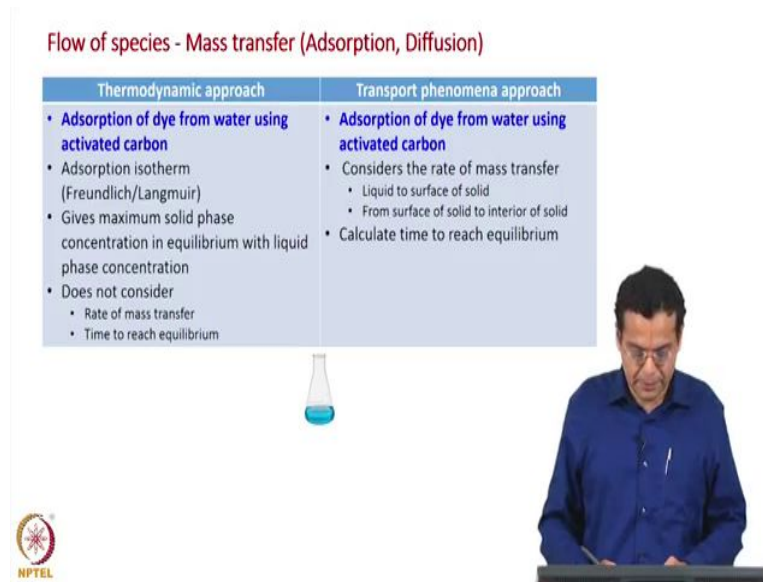
So, rate of mass transfer is not considered, that does not consider the height of the column, the direction of flow something similar to heat exchanger. Now, if you use the transport phenomena approach, you consider the rate of mass transfer; that rate of mass transfer depends on the difference between actual concentration and the equilibrium concentration, that determines the rate of mass transfer between the two phases. Moment you take this rate into account you can find out what is the height of column required to achieve a desired percentage removal. Let us say you want a 90 percent of removal then what is the height of column packed column required.

And, you can also find out the actual concentration of ammonia and the gas and liquid phase, just like heat exchanger we can find out is a co-current mode or counter current mode better. So, something analogous to our heat exchanger there we had area, length of pipe; here we had height of column. There we had accelerated temperature profile, here you have concentration profile. Once again there we can analyze the relative direction of motion of fluids, here again we can do that.

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Flow of species - Mass transfer (Adsorption, Diffusion)

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none">• Adsorption of dye from water using activated carbon• Adsorption isotherm (Freundlich/Langmuir)• Gives maximum solid phase concentration in equilibrium with liquid phase concentration• Does not consider<ul style="list-style-type: none">• Rate of mass transfer• Time to reach equilibrium	<ul style="list-style-type: none">• Adsorption of dye from water using activated carbon• Considers the rate of mass transfer<ul style="list-style-type: none">• Liquid to surface of solid• From surface of solid to interior of solid• Calculate time to reach equilibrium



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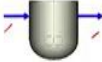
Another example, very practical example related to wastewater treatment, suppose if you have a colored water and then we want to remove color from that using an absorbent like activated carbon. So, what can thermodynamics tell us? Thermodynamics can tell us what is the maximum concentration in the solid phase, if you allow it to equilibrium which means very long time the solid phase and the liquid phase this is in equilibrium. You can find out what is the maximum concentration in the solid phase.


Once again does not consider rate of mass transfer, how long it takes equilibrium is not in the scope of thermodynamics. Come to a transport phenomena approach you consider the rate of mass transfer. Now, mass transfer takes place from the bulk liquid, it has to reach the solid surface and then from the surface to the interior of solids. These rate of mass transfer of these two steps are considered and you can find out what is the time required to reach equilibrium.

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Reactor

Thermodynamic approach	Transport phenomena approach
<ul style="list-style-type: none">• Reaction carried out in a reactor at given T and P• Maximum possible conversion<ul style="list-style-type: none">• Irreversible ~ 100 %• Reversible• Does not consider<ul style="list-style-type: none">• Kinetics of the reaction• Time of contact between the reactants/time available for reaction in the reactor	<ul style="list-style-type: none">• Reaction carried out in a reactor at given T and P• Calculate the actual conversion depending on<ul style="list-style-type: none">• Kinetics of reaction / rate constant ✓• Volumetric flow rate of reactants ✓• Volume of vessel/ weight of catalyst ✓• Contacting (fluid flow pattern) ✓





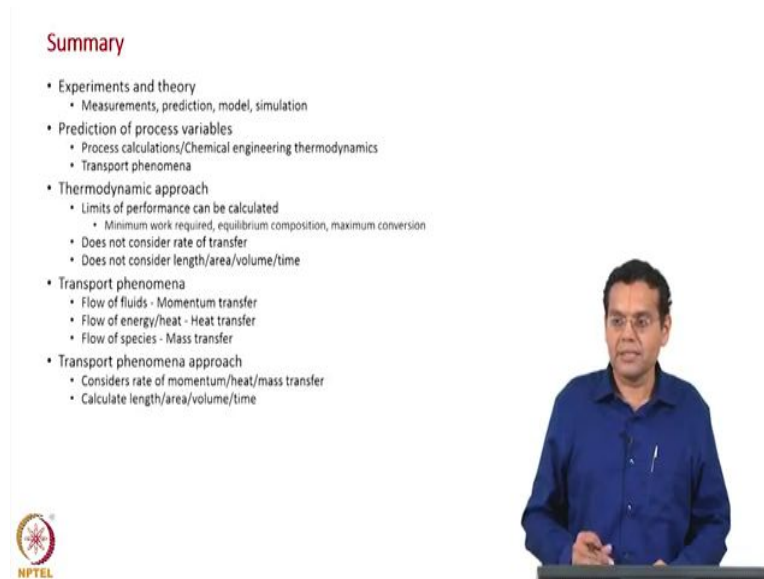
So, rate of mass transfer helps us to find out what is the time required to reach equilibrium. Just one example from the reactor, suppose we carry out a reaction in a reactor at a given temperature and pressure. What is shown as an example of a reactor where you have inflow and then outflow and let us say we carry out a reaction in this. So, analyze this thermodynamically and we can find out the maximum possible conversion as we have seen earlier. If it is irreversible reaction, it is 100 percent and if it is reversible some limited conversion possible.

Thermodynamics does not consider the kinetics of the reaction, it also does not consider the time of contact between the reactants. What is the time available for the reaction in the reactor, how long they spent time by the reactance and the reactor. All these are not considered in arriving at the conversion. In fact, for thermodynamics there is no size at all, We cannot draw even equipment based on thermodynamics. It is just a presentation by a box, there is no size attached to our equipment.

Come to the transport phenomena approach, you calculate the actual conversion. How do you calculate the actual conversion? First you take that kinetics of the reaction, include the rate constant and etcetera. Also consider the volumetric flow rate of the reactants, consider the volume of vessel or weight of a catalyst. And, also the what is the fluid flow pattern inside the reactors also considered in arriving at the conversion. So, transport phenomena approach arise with the actual conversion compared to the maximum value predicted from a



thermodynamic approach. It considers the kinetics, flow rates, the volume and the contacting pattern.

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Summary

- Experiments and theory
 - Measurements, prediction, model, simulation
- Prediction of process variables
 - Process calculations/Chemical engineering thermodynamics
 - Transport phenomena
- Thermodynamic approach
 - Limits of performance can be calculated
 - Minimum work required, equilibrium composition, maximum conversion
 - Does not consider rate of transfer
 - Does not consider length/area/volume/time
- Transport phenomena
 - Flow of fluids - Momentum transfer
 - Flow of energy/heat - Heat transfer
 - Flow of species - Mass transfer
- Transport phenomena approach
 - Considers rate of momentum/heat/mass transfer
 - Calculate length/area/volume/time

So, that brings us to the summary of the first part of introduction. We started experiments and theory, looked at measurements which you would like to predict using a model which you call a simulation. And, prediction of process variables either based on thermodynamic approach or transport phenomena approach. Process calculation course just a subset of thermodynamic approach. The thermodynamic approach tells us the limits of performance, gives us minimum work required, equilibrium composition, maximum conversion.

Does not consider rate of transfer?, be it, heat transfer, mass transfer, momentum transfer and length, area, volume, time are all not at the scope of thermodynamics; all those are not considered. We saw transport phenomena deals with flow of fluids which is discussed under momentum transfer. Flow of energy or heat which is discussed under heat transfer and flow of species discussed under mass transfer. What is scope of transport phenomena approach? Considers the rate of momentum, heat, mass transfer because, of that we can calculate the dimensions namely length, area, volume, time is also brought into picture.