Aspen Plus Simulation Software – A Basic Course for Beginners

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Lecture-29
Absorption and Distillation - Part 1

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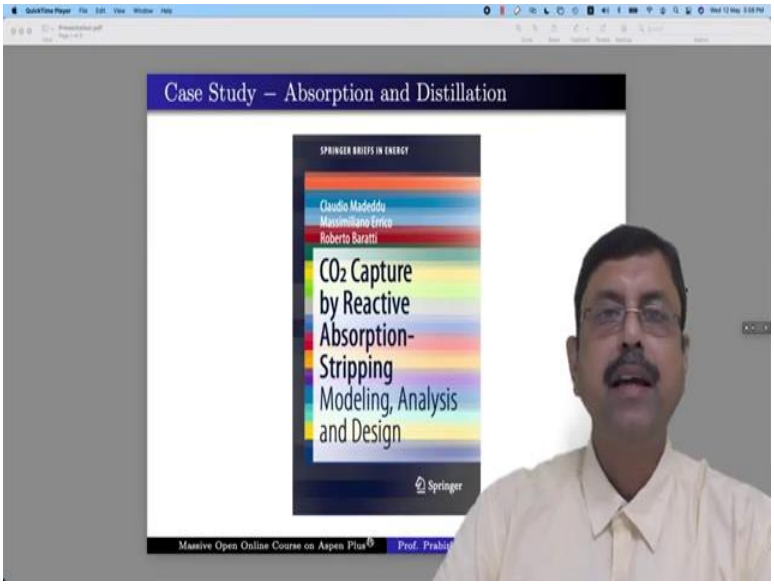

Welcome to the massive open online course on Aspen Plus. In this week we are supposed to perform a case study; 2 case study in fact one is on absorption the other one is on distillation or stripping. Now I have chosen a problem in which both these unit operations can work together. Individually we have learned these two unit operations in other case studies which we have performed earlier but in this particular case study we shall take reaction mechanism into these unit operations.

In other words, it will be reactive absorption and stripping. Now the case study that I have chosen here is from this book CO_2 Capture by Reactive Absorption and Stripping Modeling Analysis and design by Claudio Madeddu Masimiliano Errico and Roberto Baratti. Now this book is available in the internet you can purchase it or you can borrow it from library if you have it. But this book is needed if you want to solve this problem.

Unlike in the previous weeks I do not have any problem statement drafted rather I will use the problem statements used in this particular book which has all the necessary information for our case study.

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So, this is the book that I was talking about it is published by Springer Briefs in Energy. Now to begin with you might be aware that carbon dioxide is known to be a greenhouse gas which is responsible for global warming. And there are various sources of carbon dioxide but most prominent source is the power plant exhaust which has flue gas.

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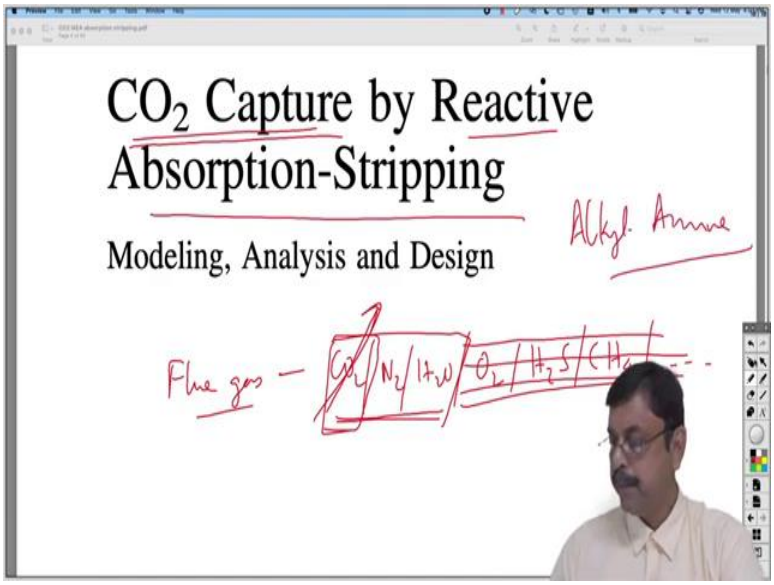

Now the flue gas is basically is a mixture of carbon dioxide, nitrogen, water vapour, unreacted oxygen, H_2S, methane and other impurities but for this particular problem we will not consider any one of them will consider only carbon dioxide nitrogen and water vapour. We will assume only these three components are there in our flue gas. Now obviously if the percentage of carbon dioxide is more in flue gas we cannot release it in the environment because it will create pollution.

We need to knock off this CO_2. Now in this book they have described a procedure to capture CO_2 by reactive absorption and stripping using alkyl amines. You might know that alkyl amines have the capability of absorbing CO_2 whenever CO_2 and amine they come in contact with each other they react and thereby the CO_2 gets absorbed in amine and it is very easy to separate them. If we heat the rich amine that means the CO_2 absorbed in amine that we call it as a rich amine if we heat the rich amine, then CO_2 gets dissolved very easily and amine gets free of CO_2 and that can be reused.

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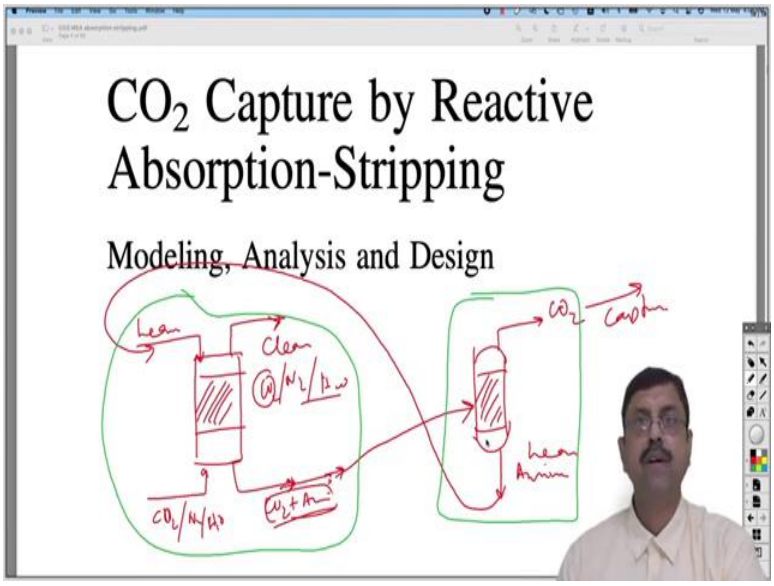

So, basically we will have an absorption column which will be a pad column flue gas is passed through the bottom. So, it will have a combination of CO_2, N_2 and H_2O and lean amine that means amine free of CO_2 will be poured from the top and they will react with each other. And the rich amine that means amine plus CO_2 mostly CO_2 will be there in compound form that will come out from the bottom of the absorption column and a clean gas that means the gas free of CO_2.

So, it will be mostly nitrogen and maybe some water vapour and there will be some unabsorbed CO_2 will also be there 100% CO_2 removal is never possible but mostly the amount of CO_2 will be very less. So, we can safely release into the atmosphere. So, we will have the rich amine over here which we need to heat up to regenerate our amine for reuse for that we will take another column which again will be a packed column we shall send this rich amine to this column and heat it. Upon heating CO_2 will come out from the top because CO_2 gas is lighter and amine will come out from the bottom as a liquid.

This CO_2 can be captured through some means I mean it will be concentrated and stored somewhere else that is the purpose basically of this system. And this amine becomes lean again because it has dissolved CO_2. So, it can be again recycled back to the absorption column. So, this is the overall process that we will deal with in the case study. Now in the very beginning we shall study only the absorption column and then we will study the stripping column and at the end we shall combine them along with some other unit operations such as pumps or heat exchanger or valve etcetera and make it a comprehensive case study.

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So, to begin with we need the list of components. Now you will see this particular book has been written keeping aspen plus users in mind and all the modeling and analysis tools that have been described in this book refers to aspen plus extensively. So, in the introductory chapter they talk about pollution due to carbon dioxide and some brief history how the carbon dioxide changes the climate and political debate along with it etcetera.

And then talk about carbon capture and storage technologies. These are not relevant to our study our actual studies begin in the second chapter where process description is given, how to set the property environment, the simulation environment. Aspen plus we will use RadFrac column for absorption and stripping as well and it will be run in rate based mode they will give the information about how the rate based simulation environment will be designed and so on.

And third chapter will talk about the model validation for the absorber the rate-based correlations liquid film discretization parameters all of them will be done. And then some segmental analysis

how the interfacial mass transfer happens etcetera. The chapter 4 deals with model validation of stripper and finally a comprehensive absorption plus stripping both together as a wholesome case study is presented in the chapter 5.

There are other economic evaluations are there that will not consider at this moment. So, we can directly go to the chapter 2, yes. So, process modeling in aspen plus. So, here the process description has been given and the simplified flowsheet of CO_2 capture by reactive absorption stripping plant. This will come later and here building the model in aspen plus although we know how to do it but they have given it in a nutshell we have to add in the components diffusion in two phases simultaneous mass transfer energy transfer equilibrium and reaction kinetics we have to refer and give the parameters in that.

Vapour liquid equilibria gas liquid equilibria we have to analyze with non-ideal thermodynamics all these factors will come in this case study. And then we have to select the property environment first components this particular figure is very familiar to you because every. Now and then whenever you begin your case study you have to give the component specification in this manner. What is interesting over here you can see other than the complete compounds like carbon dioxide water monoethanol amine etcetera.

You also have some ions like CO_3^{2-}, it is an ion which has been given as a component because ionization will take place there are reactions that will happen in reactive absorption where CO_3^{2-} ion or H_3O^+ ion or HCO_3^- ion they will be produced. So they have to be inserted in the component list in order to run the simulation properly. And these are the stoichiometry that has to be inserted in the simulation window and this is the process flow sheet will come to it later. So, these are the chemical reactions.

So, all together we will have a set of three ionic equilibrium reaction that is reaction one two three 2.1, 2.2, and 2.3 these are ionic equilibrium reaction and there will be two kinetic reversible reactions involving CO_2. So, we will have these two kinetic reaction and these three ionic equilibrium reactions which we have to insert in the reaction list. And where do we get the

parameters from? They are also obtained from various sources like number 6 number 11 these are references.

For instance, the kinetic constants for equation 4 and 5 that is these two equations involving CO_2 they are obtained from these two papers 18 and 32. So, paper 18 is here from applied energy published in 2016 and 32 being sent its relatively old paper published in 1956 in transaction of Faraday's society. So, aspen RadFrac model, RadFrac model is used for this absorption and stripping columns.

So, we have to use red track column they can be run in equilibrium stage mode or rate based mode we will use it in red best mode this is the rate-based segment representation of the absorption this is a well-known figure which you will find in any mass transfer book and mass transfer occurs with various theories. And you have to choose the correct theory and it is rate equations in order to run the simulation properly. This model are based on true film theory of Lewis and Whitman.

Now if you want to know further into two film theory you should refer to this particular reference and film modeling resistance, film ordering liquid film discretization everything has been said over here. Now you will come across reaction condition factor, film discretization ratio number of discretization points in the film these are the few topics that we will come across while running the simulation.

So, this will come later first let us go to the aspen plus simulation window and start preparing our simulation. This particular simulation involves lot of components and lot of reaction mechanism. So, what I have done I have already included those components and reaction mechanism into the simulation file because there is nothing to teach over there you already know how to enter the components you already know how to enter the reaction mechanism.

So, I just wanted to save some time and done those preliminary works myself without waiting for this lecture I will obviously show you the final result but those things have been done let me go to the simulation window first yeah. So, this is the simulation window. Now you have all the components selected that is mono ethanol, amine, water, carbon dioxide, hydrogen sulphide. Now

you may ask me why hydrogen sulfide because hydrogen sulfide may be present in flue gas as an impurity obviously not in large quantity small quantity may be.

So, in future if you want to change your simulation environment if you want to add in a few impurities if hydrogen sulfide is present in the flue gas if you want to add certain number of equations more due to those impurities then it will be easier for you. You do not have to add the components again and re-run the property method. So, these things I have already added in if you use it. It is if you do not use it does not matter it will just stay over here.

So, this is the comprehensive list of components that you can use for CO_2 sequestration. Property method we will use ENRTLRK that is electrolyte nrtl model with Readily Quanks equation of state and Henry's law. What are the Henry's components you will find over here. So, we have this Henry's component. So, these are the selected Henry's component in the problem and this is the chemistry for mea you will find them over here this one. We have to add in this stoichiometry and we have done the estimation in which I said that estimate all missing parameters.

And the result run status; it says calculations are completed normally on this date and this time. Now we shall go to the simulation window. In the simulation window we have to add in three ionic equilibrium reactions and two kinetic reversible reactions. So, for that I have already done that meah reactions you will find this three ionic equilibrium reaction and two kinetic reactions which are reversible in nature.

So, this one is forward reaction and this one is backward reaction for this also it is the forward reaction this is the backward reaction. And if you want to know the equilibrium constants I have asked them to compute the equilibrium constant from Gibbs energy for all of them. There are three ionic equilibrium reaction for all three I have asked them to calculate from Gibbs free energy but kinetic equation we cannot do like that.

We have to use the power law which I am using over here with this particular parameter that we have found from the references that I just mentioned one is from applied energy by Erico and another is from Faraday's society by Pinkscent it is an old paper as far as remember it is 1956

paper. So, from there we have gathered the data and added. So, if you want to know the data this is the fourth reaction it is the first kinetic reaction.

The second kinetic reaction is this one is that the data third kinetic reaction will be like this and the fourth kinetic reaction will be this. So, these are the four reactions we shall use it where it is needed. Now let us open the flow sheet. So, this is the main flow sheet we have to add a column first. So, Radfrac we use a packed bed column let us increase the size a bit name it as ABS this is the flue gas in, this is lean amine in.

Lean amine means the amine without any CO_2 in it fresh amine in other words and this will be the gas out which will be clean gas that means this gas will not contain any significant amount of CO_2 and this is the rich amine that is amine filled with CO_2. We rename them accordingly we say this is LEAN this one is FLUE this is RICH and this is CLEAN gas. Now press next. So, it is asking for the specification of the flue gas. So, for that let us go to the chapter 3 yeah model validation for the absorber.

So, there are two selected runs for feed characterization one is by Tontiwachwuthikul et al and the other one is Razi et al. Now we can choose either of them but for this case study let us choose this one. When you do the practice you can do it with Razi et al tool also. So, we will choose this flue gas. So, it is 288.15 Kelvin and pressure is 103.15 kPa. So, 288.15 it is 288.15 Kelvin and 103.15 kPa and molar flow rate is 0.14 mol/s and the composition mole fraction is 19.1% CO_2, 10% water and the rest nitrogen.

So, we have 0.191, 0.1 and into 0.709 total 1. So, flue gas done then it will ask for lean I mean yes lean amine it is 292.15 Kelvin, pressure is same 103.15 kPa and flow rate 1.04. So, 1.04 mol/s and composition it is 5.5% mea and 94.5% water. So, this is mea and this is water. So, lean amine also has been specified. Now, the absorption column. So, for absorption column it will be rate based number of stages has not been given.

So, we can choose any number of stages we can choose say 15 stages or 30 stages and it is an absorber. So, we do not have any condenser or reboiler. So, condenser none and reboiler none

streams flue gas has to be sent from the bottom and lean amine will be poured from the top. So, flue gas at 30th stage or on 30th stage because the stages will be counted from the top, top stage is 1 then 2, 3, 4, 13th stage is the bottom stage and lean amine will be poured above the stage one here the clean gas or clean vapour will go out of the stage one and rich amine will pass through the stage 30 as a liquid.

Pressure they have not said anything about the pressure at the stage 1. Let us keep the pressure at the stage 1 as 103.15 kPa because lean amine is being inserted from the stage one at that pressure. So, just to keep a parity will keep as 103.15. So, 103.15 kPa. So, specifications have been given. Now as it is a rate based column. So, we have to enter the column internals. So, go to column internals add new. So, add a new section let us keep only one section in the column.

So, it begins at stage 1 ends at 30 the sizing will be rate based, it will be a packed column, packing type. So, information has been given it should be 12.7 mm Berl Saddles. So, we look for Berl Saddles yeah this one it is Berl Saddle and automatically the vendor has been chosen there are many vendors. Now all those vendors they have their different but we have to choose a dimension which is 12.7 which gives 12.7 because it has been said 12.7 mm Berl cells.

So, Norton does not have it, Gliss it also does not have it whatever generic none of them has exactly 12.7. So, let us choose 13 mm. So, that is the closest one and we will keep the default one only let us not change it packed height it is 6.55 m. So, we will write 6.55 m and diameter is 0.1 m. So, it is done. Now we shall come down to rate based modeling. So, here we have to add in a few information a few minutes back, I was discussing about what they were asking for.

They have given some information about how to choose the rate based correlations and they said that the mass transfer coefficient has to be calculated from this particular paper Onda et all and heat transfer coefficient from Chilton and Colburn analogy. Now if you go to this section first of all you have to click this rate based calculation once it is done this is open for you must transfer coefficient method there are various methods available.

Now they have asked you to choose Onda et al, 9. So, this is the paper Onda et al 1968 mass transfer coefficient between gas liquid phases impact column, Journal of Chemical Engineering, Japan. So, Onda 68 they have chosen Onda 68 by default. So, we will keep it if you have something of your own you can use it as user based but then you have to supply the model. Now heat transfer coefficient they have said you can choose the Chilton and Colburn analogy.

So, by default is there as Chilton and Colburn analogy interfacial area method it is again Onda 68 weighted surface area Onda 68 and some further information is given liquid film discretization parameter. So, a reaction condition factor was set to 0.9 in order to give more weight to the bulk condition in the evaluation of film reaction rate. Due to the first reactions in the liquid film what is reaction condition factor and how it is helpful for your simulation setting up.

You can go through the work of Zhang et al and then you can find it. For the time being let us go to the simulation and look for reaction condition factor and put 0.9 over here um after significant number of simulation it was found that 5 non-equidistant discretization points in the liquid film were sufficient for correct description of the profiles and this value is in agreement with work of Kucka et al. So, for film discretization first we will say the liquid phase film should be discretized and that it will ask for number of discretization point will say 5 because that has been found to be the best.

For vapour phase we will also consider the film and then film discretization ratio was fixed at 10. That was found to be a good compromise between discretization points placement and discretization steps for the numerical solution of the system. So, we shall look for film discretization ratio and put it as 10. All other things we can just keep it as it is. So, even without that the simulation is ready for run.

So we just run it we have got some problem and I believe the problem lies over here yes. So, at many places you will see the operating points are lying over here. So, many places are getting dried up. So, our liquid flow rate or amine flow rate is very very low. So, we will increase the flow rate of a mine. So, we just open it instead of 1.04 let us make it 3.04. So, it has been increased almost three times if not exact.

So, there is some more problem over here let us see what problem we have encountered. We have forgot to add the reactions although we have defined reaction but we forgot to add it. So, we will say stage 1 to stage 30 we will have reaction id of mea reaction mea reaction has been defined over here this is a mea reaction few minutes back I told you. So, that mea reaction will be active from stage 1 to stage 30 and also in the red based modeling we include the mass transfer rate in the report option.

Now run it once again. Now it has converged. So, we are happy that we have a convert solution and first thing first we shall first save this simulation because every time you have a converse solution make it a habit to save it because you never know where your solution will go wrong. So, if your solution goes wrong and you are not able to come back to the point where you have missed you can begin your simulation from the saved simulation you do not have to start from the scratch.

Now at this moment let us see the stream results. Now let us compare the mole fraction. So, we have in the lean gas we had 94.48% of water the percentage has increased in the rich gas because a considerable amount of water that was there in flue gas that has come to the amine. And from nearly 10% of flue gas it has reduced to 2% CO_2 it was 19.1% reduced to 0.38% in clean gas. So from flu to clean the CO_2 has almost gone and rich amine is having that amount well you may argue that this is not the figure which can come because 10^{-9}.

So, amount of CO_2 may not be. So, less in rich amine yes definitely we will explore it how for that you have to see the mass flow rate here you see in the flue gas we had 4.23656 kg/hr of carbon dioxide and in clean gas it is 0.06 2 kg/hr. So, almost 4.17 kg/hr of CO_2 has been taken by the amine. But in rich amine we have very less amount of CO_2. So, where is the CO_2 where has it gone it has gone to HCO_3^- it has gone to CO_3^{2-}, also it has gone to $MEACOO^-$.

So, CO_2 is mostly in ionic form not in CO_2 compound form. Now let us check the profile of the liquid temperature. So, for that let us change it to Kelvin. Now we have to compare it with this one here they have given the liquid temperature versus distance from the bottom. So, this is at the

bottom and this is at the top definitely at the top the temperature will be lower and at the bottom temperature will be higher.

So, we should have this kind of graph so let us see whether we get it for that let us copy it and go to excel file. Now this is stage 1. Now the height of the column is 6.55 m and we have 30 stages. So, each stage is 6.55 by 30 m of length. So, cumulatively this into this is the length of stage 1 this is the length of stage 1 and 2 together this is the length of stage 1, 2, 3 all together likewise 6.55 is the length of all 30 stages together. So, distance from the bottom will be 6.55 minus this for everything.

So, this is the distance from bottom this is distance from bottom this is distance from bottom and so on. So let us insert one scatter instead of stage one we will keep this. Now this particular graph is not looking like this one why because we have we have got the lean amine flow as 3.04. Now if we run it once again with 2.04 it has converged then try with 1.04 the original figure this time it has converged column hydraulics may not support us to some extent it is running anyway let us go to the profile once again and copy go to the excel file press it yes.

Now we can see the temperature well we have forgotten to change it to Kelvin. So, copy, once again press it over here. So, make it 20 make it 20 yeah it looks better. So, the trend is the same, it begins somewhere near 320 ends somewhere near 290. So, it is the same trend what about CO_2, vapour composition. So, for that we have to go to the composition vapour then mole and CO_2, copy press it here instead of this one yes. So, it begins somewhere 0.2 and ends very near 2.01 or something.

So, begin somewhere at point two and end somewhere at point one point zero one rather. Now if you want to see the CO_2 interface flow rate for that we have to go to rate based modeling interface profile mass transfer unit mol/s. So, copy this one press. So, instead of this one like this yeah so, this is the bell-shaped curve yeah trend is identical this is H_2O interface flow rate. So, this is the H_2O file instead of this one yes.

So, the trend is similar. Now if you change it to say from 30 stage; to 90 let us see how it changes. Now for that what we need to do is we need to change the setup from 30 to 90. So number of stages 90 lean amine is entering on stage 90 and then the reaction it is happening up to stage 90 and the column internals the section is up to 90 then run it once again. We have some results with us especially we are interested to know the profile device profile rather for 90 stages change it from centigrade to Kelvin, copy place it over here.

So, instead of 30 will say 90 because we have 90 stages all others will remain same. So, we shall add one more plot over here. So, for us this is the x-axis and y-axis is this one. So, you can see the new line red line it has gone up similar trend is observed over here for 30 it is somewhere here but for 90 it is going up and over here. So, after 1 meter the profile for 30 stage column it is higher than a 90 stage column.

You see over here after nearly 1 meter the profile of a 30 stage column is higher than a 90 stage column. If you find difficulty to understand it properly you can shift it to a chart. So, this one is very much similar to this one. So, this one will also be similar. So, that is how we do the rate based modeling of absorption column or reactive absorption of CO_2 in monoethanol amine. So, the purpose of 90 stages column is over we have done the analysis.

Now we shall go back to 30 stage column why because unnecessarily it is not wise to carry on with a 90 stage column because it will take a lot of computational effort and for each and every run there is no need to put on such a computational load on the computer and increase the time of convergence and that is the reason we are going back to 30 stage column. We are done with the absorption column. Now we will shift to the stripping column you.

(Video Ends: 56:44)