Basic Principles and Calculation in Chemical Engineering
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Module-10
Lecture-31
Numerical Integration

Welcome to massive open online course on basic principles and calculations in chemical engineering. So, we are discussing about the computational techniques under the module 10. And in this lecture of module 10 I will discuss about numerical integration with examples.

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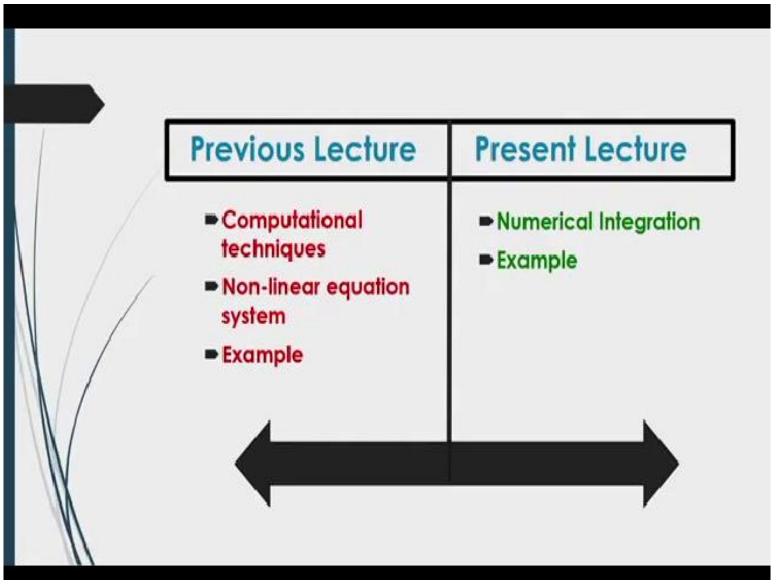

In the previous lecture we have described nonlinear equation and how to solve that nonlinear equation with examples also you have described in our earlier lecture that how to you know free to that linear equations with experimental data by least square method. So, here this lecture is basically continuation of that, you know, computational techniques. In this case, how to actually calculate the integration from the, you know discrete data of some you know, variables.

And what will be the integration of those profile of discrete data and what will be the area under that you know profile based on the integration value how to estimate that and how to calculate that, what are the different you know, rules are there to calculate that, you know area under the curve by you know numerical integration. So, we will discuss here.

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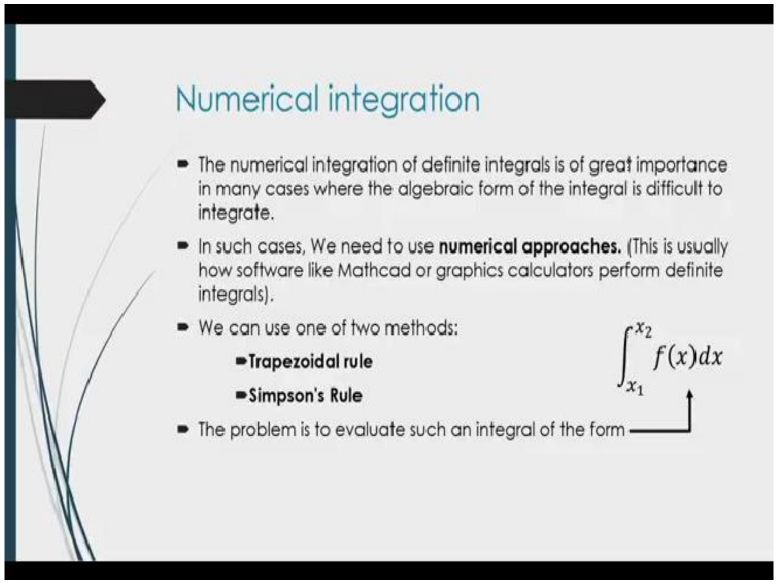

So, the numerical integration of the you know definite integrals, you know is of great importance in many cases where the algebraic form of integral is difficult to sometimes integrate there. So, in such cases we need to use numerical process. This is usually how software like you know mathcad or graphics are calculator perform definite integrals there. So, we can use 1 of the 2 methods here like trapezoidal rule and Simpson's rule.

The problem is to evaluate such an integral of the form like this here instead that time like x 1 to x 2 of the function, you know f of x. So, we can see that this how this you know, integration within limits of x 1 to x 2 can be you know numerically calculated.

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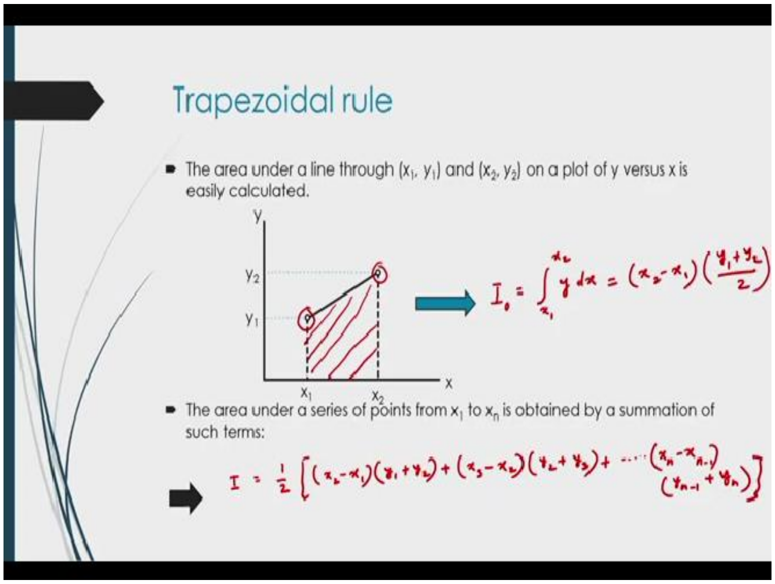

Now we told that there are 2 methods to calculate the you know, integrals here from the data within range of x 1 to x 2 1 is called trapezoidal rule. Now, based on these the area under a lines through here x 1, y 1 and x 2 y 2. So, this is the you know line between these 2 points. Now on the plot of this y versus x axis, you can calculate what should be the area under this line like this, this area how to calculate you know here.

So, this you know area under a series of points from that, you know x 1 to x n here, here up here in this picture it is x 1 to x 2, but you may have you know x 1 to x n value and it can be obtained by summation of such terms here.

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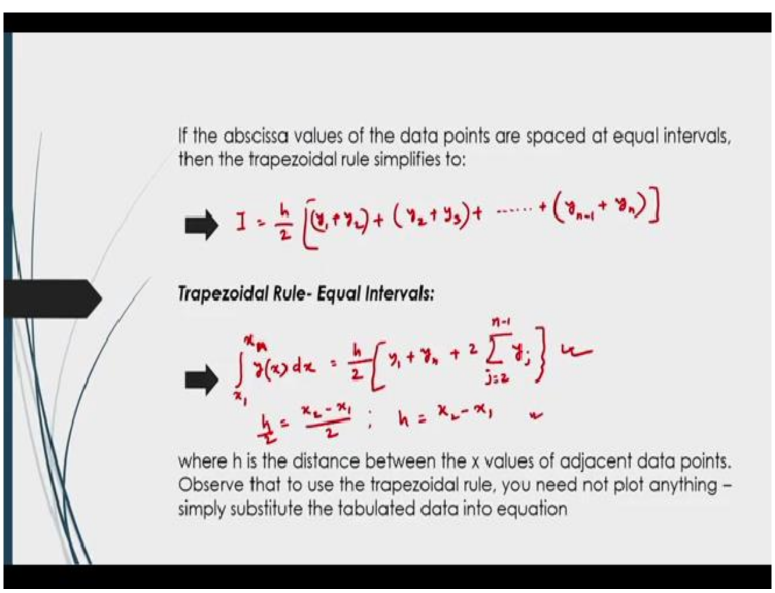

In this case let us see that thinks now we will see that in this case this integrals can be you know, obtained by this formula as per trapezoidal rule. So, this will be equal to you know, here x 1 to x 2 here function is y into dx. So this is your integrals. So, from this you know we can you know from this limit of the x 1 to x 2 data and corresponding value of y 1 and y 2 data we can obtain this area under this you know grabbed by this, you know, definition of the integral says like here it will be you know that x 2 - x 1.

This is here x 2 - x 1 into here, y 1 + y 2 divided by 2. So, by this equation you can get this you know that what we the area under the curve, here x 1 to x 2 this is the limit of this you know x value whereas y 1 y 2 is this is basically functions value at this x 1 and x 2 and then you have to take it an average. So, from this you can get what should be the integrals there. Now area suppose under the series of points, from x 1 to x n that can be obtained by summation of such terms like here that can be written as here I as these.

So that will be is equal to here we can write 1 by 2 into here, x 2 - x 1 into y 1 + y 2 and then plus then x 3 – x 2 like this into y 2 + here y 3 then + dot dot dot, x n here we can write here x n - x n - 1 into here we can write y n - 1 + y n. So, from this equation you can obtain of what will be the you know, area under a, you know you know line within you know point here, where x 1 to x n. So, this is called trapezoidal rule.

Now, if the abscissa values of the data points are you know spaced at equal intervals then the trapezoidal rule can be simplified like this here, we can write this I = h by 2 into you know y 1 + y 2 + y 2 + y 3 + dot, dot, dot we can write up to here y n - 1 + y n. So, from this if abscissa value of the data points are spaced at equal intervals, then this trapezoidal rule will be simplified to this.

Now, if you are having that you know equal intervals, so, we can write this integral as here suppose, x 1 to x 2 y you know as a function of x into the d x. So, that will be is equal to h by 2 here we can write y 1 + y n + 2 into summation of here you can write j = 2 to here n - 1 into y j. So, this is your generalized form or h is the distance between the x values of at just in data points. That means here we can write here, what is the difference between these 2 points x there like s that will be is equal to if there is an equal intervals you can write x 2 - ~~you know~~ x 1 divided by 2 this is your, you know h value.

So, here h is the distance between no this is h by 2 that will be x 2 - x 1 by 2 that means here h will be equal to simply x 2 - x 1. So, this h is the distance between the x values are adjusting data points that you know observed to use the trapezoidal rule. Now, in this case you need to plot anything simply to substitute tabulated data into the equation there. So, in this way you can calculate.

So, by this equation, you can calculate what should be the integrals here, in this case, we can write that this limit will be x 1 to x n instead of x 2 here. So, because here we are considering that n number data whereas for 2 points x 1 and x 2 we have discovered that this will be equal to simply this equation by this equation that 2 points you can get this integrals, but n number of points that you have to use this equation and in general you can write this equation here.

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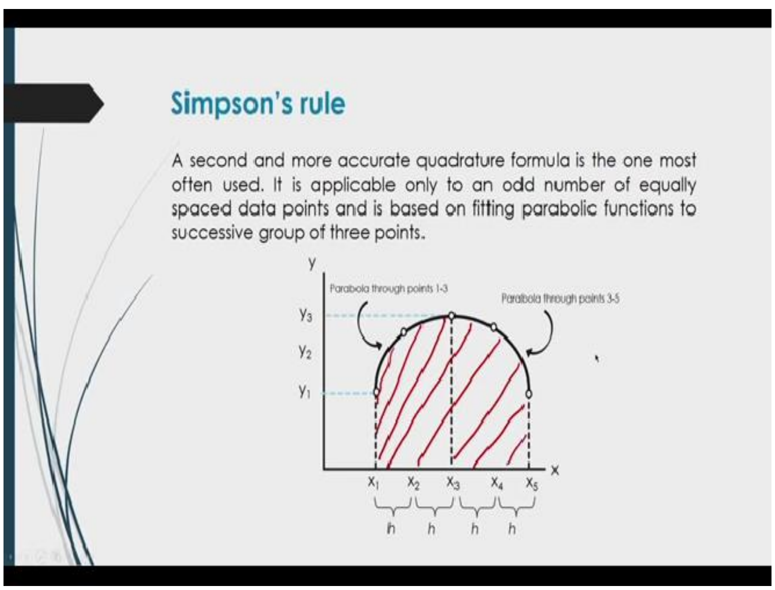

Another method is called Simpson's rule. Now, in this case, you know, this is, you know, more widely used, you know techniques to you know estimate that integrals within a certain limit, it is applicable only to an you know, odd number of equally spaced data points and is based on fitting parabolic functions to successive groups of 3 points there, like here we will see that one you know parabola, 2 points here, 1 to here 5 like this.

And in the left side 0.123 and right side to be parabola at 2.32 and in this case, you will see that, if we you know, divide these x axis into equal intervals, like this like h here x 2 – x 1, and here again, h is x 3 – x 2 x 4 – x 3 x 5 – x4, this will be your h value. Whereas the y axis you will see that for each value of x 1 you will get that function value as y 1 and similarly y 2 y 3 like this and based on this you know that you know parabola.

And under this parabola what will be the area that can be obtained by this you know integrals and that integrals can be calculated based on this you know Simpsons rule.

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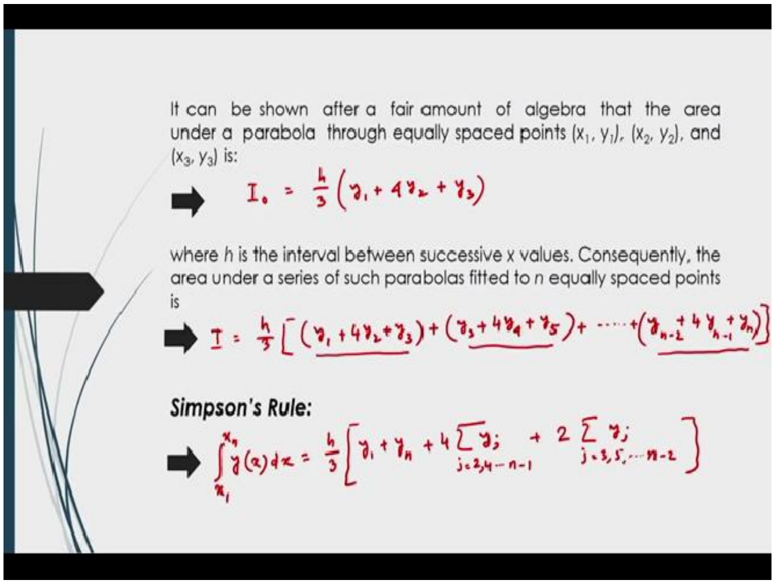

Now, what is that Simpsons rule it can be actually shown after a you know fair amount of algebra that the area under a parabola through equally spaced points of x 1 y 1 x 2 y 2 and x 3 y 3 can be actually expressed as here, I 0 that will be h by 3 into y 1 + 4 y 2 + y 3, if you are having 3 points here, so, it can be represented by this you know equation. In this case h is the interval between that successive x values consequently the area under the series of such parabolas you know fitted on that on the value of that x 1 to you know x n.

And n number of values will be there, those are equally spaced points and that can be expressed by this integral as I will be is equal to here h by 3 we can write here similarly y 1 + 4 y 2 + y 3 and then after that here again, the same, you know, pattern will be starting from y 3 like this y 3

+ 4 y 4 + y 5 like it will be continued up to a point you know n here then final point will be coming as here like this, y here n - 2 + 4 into y n - 1 + here y n.

So, this is your general term to express that integrals, if they are you are having n number of you know of data for this you know functions as far that the number of data of x 1 to x n. In this case here you have to find out as far in the h value and then successively you have to you know, consider this pattern here y 1 + 4 y 2 + y 3 and then other points like this y 3 to y 5 which will be y 3 + y 4 + y 5.

And then you know up to nth value you can consider by this you know general value. So, we can write this the Simpsons rule here as a general form like this integration of your suppose x 1 to x n for the function y as a function of x into d x. So that can be written as h by here 3 here we can write y 1 + last point is y n and then plus here 4 into summation of who can write y j here, j will be is equal to you know that 2, 4 dot dot dot dot here up to n – 1.

And then plus, then 2 into we can write summation of here you can write j is equal to you know 3, 5, dot dot dot here n - 2 and then here it is y j. So, based on these, you know, formula you can calculate what should be the integral you know or area under that n functions that is represent in the graphical form. So, this way you can you know obtain the integrals based on The Simpsons rule.

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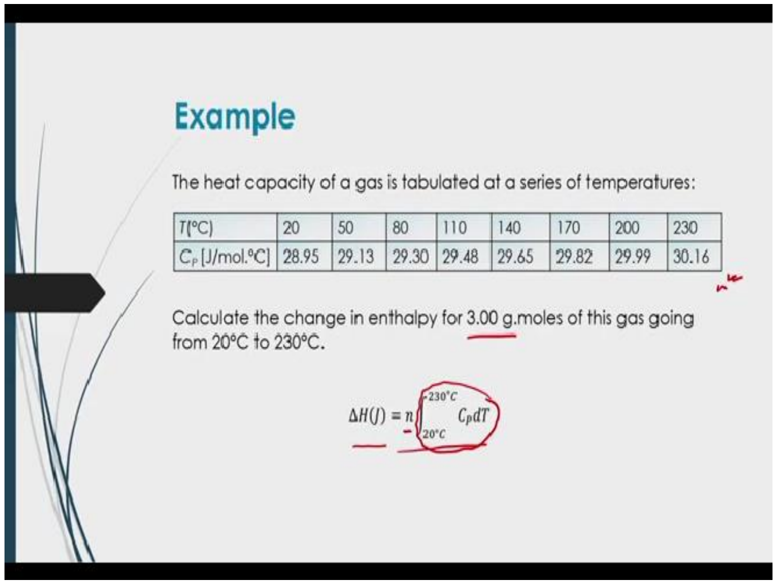

Now, let us have some examples here to calculate based on that theory. Now, one example is given that the heat capacity of a gas is terminated at a series of temperatures like this T in degree Celsius like 20 50 80 110 140 170 200 and 230 and specific heat capacity is given like where at 20 degrees Celsius it is 28.95 and at 50 degree Celsius it is 29.13 and at 80 degrees Celsius it is given 29.30 and 110 will be 29.48, 140 it will be this, and 170 up to 230 you are having these saw you know specific capacity value.

Now you are having here the data like 20 to 230 degree Celsius within this range this specific capacity data you know are having. Now, you will see that this temperatures are a difference that is successive temperature differences, you know on the 30 degree Celsius. So, with us you are getting that you know 20 to 50 then 50 to 80, 80 to 110 and 110 to 140 like this, everywhere you are getting that interval is same.

So, equal intervals is there and here number of points are like 1 2 3 4 5 6 7 8 point. So, here even number of points are there. So, how to solve this problem to find out the change in enthalpy for you know 3 gram moles of this gas that is going from 20 degrees Celsius to 230 degree Celsius. So, here enthalpy can be calculated based on this equation here given that is equal to n into integral of 20 to 230 degree Celsius into C p into dT.

Now, this n is you number of moles here it is given that 3 gram moles of this gas and also here it is given that the integrals value will be you know C p to dT. So, total enthalpy change will be n into here, like this 20 to 232 into C p dT. Now this part is your integral that you have to obtain based on this you know data given in the table. Now, how to actually apply that you know trapezoidal rule or Simpsons rule to calculate this, you know enthalpy based on this.

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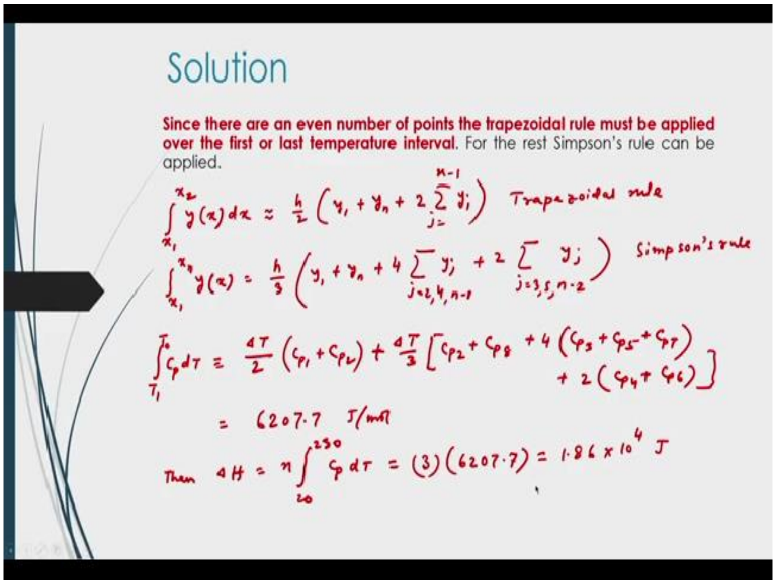

Now, in this case remember this since there are even number of points the trapezoidal rule must be applied to what the first or last impressive interval, this you have to remember, because, where Simpsons rules in early applied for you know that you know that odd number of data and to get that similar pattern of that you know successive 3 points to find out that you know that integrals and here since we are having you know, 8 points, so, here even number of points.

So, the trapezoidal rule first you have to apply over the first or last in intervals and for the race to Simpsons rule can be applied there. So, according to this, you know, we can then write here this according to trapezoidal rule what we can write here for first you know 2 you know points that is here 20 to 50 within this range of temperature we can write that integrals here x 1 to here x 2 + 2 points we can write here y into y as a function of x into dx that will be is equal to h by 2 here y 1 + y n + we can write here 2 into submission of here j = you go 2 to n – n – 1 that is y to j.

So, this is your basically trapezoidal rule. So, and for Simpsons one third rule we can write here x 1 to here x n we can write y as a function of x that will be is equal to h by 3 into what is that y 1 + y n this is your general formula 4 into summation of her j = 2, 4, n - 1 here and then y j + 2 into submission of j = 3, 5, n - 2 here y j. So, this is your you know Simpsons rule. So, as for this problem we can write here then the limit here T 1 to T you know that final that is your T 0 that means here C C p into dT.

So, in this case we can write delta T by 2 here delta T here, this is h that means here temperature difference, then we can write here C p here 1 that is first value of C p 1 + similarly, C p 2 second point here specific capacity, this is your trapezoidal rule as for that and plus then, you know delta T by 3 this part will be applied for Simpson rule. So, it will be here, like C p here we can write 2 + C p, you know who that C p 2 + here we can write C p 8 here then plus 4 into C p 3 + C p 5 + C p 7.

Then we can write + 2 into here, C p 4 +C p 6. So, this is your final equation as per this you know, combination of this you know trapezoidal rule and Simpsons rule. Now, substituting the value of this, you know, here delta T and then C p1, C p2, all those values then we can get this will be around 6207.7 joule per mole. So, this is your you know that integral forms of that equation for this enthalpy here, that is delta H that will be is equal to n into this.

Now, total enthalpy can be calculated based on these as then we can calculate delta is H that will be is equal to here given n what is the you know temperature here at 22 to 30 20 to 230 into C p dT, so, that will be is equal to here n is given to you, that is 3 moles and then integral value is opted here as 6207.7. So, finally to becoming as here 1.86 into 10 to the power 4 that means here joule. So, this is your final answer for this.

So, by this you know point we can then calculate what should be the integrals and then what will be the enthalpy. Now, let us do another examples here.

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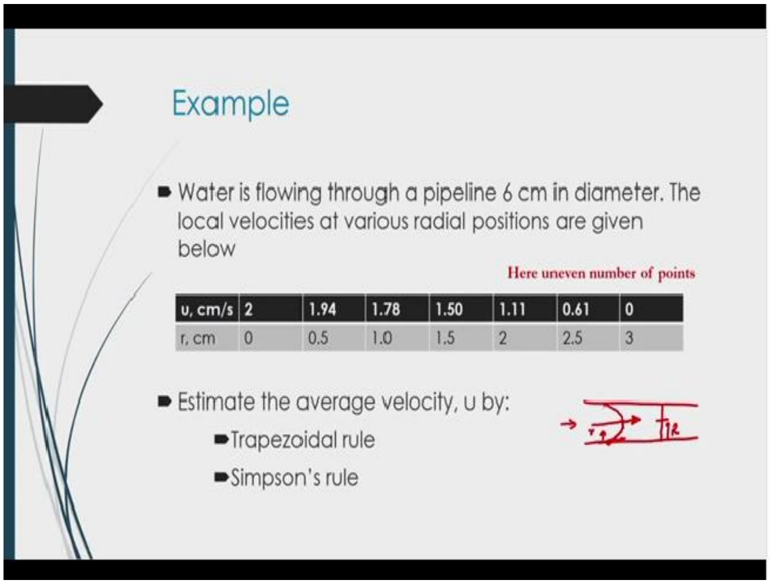

Let us consider that water is flowing through a you know a pipelines that is 6 centimeter in diameter and the local velocity at various you know radial positions are given below here like as per this tabulated form here at radial position of despite suppose this is your pipe and the fluid is that is your water is flowing. Now at different radial position you will see that velocity will be changing .

Because here this velocity to be like this, this velocity profile will be like this. Now, at the center that velocity will be higher, whereas at this you know adjacent to this wall the velocity will be lower. So, whenever this radial position will be there, according to this radial position this velocity of this you know water will be changing. Now, according to that, we can have this data experimental data like this.

At you know R = 0 that means, at this wall, this velocity will be equal to what this will be equal 2 or as this at 0.5 this R that is 1.94. And here, you know set at R = 1 is 1.78 at 1.5, 1.50 and then R = 2 it is 1.11 and 2.5 it is 0.61 and at 3 it will be again 0. Now, based on this, we can write here this, you know average velocity and that average velocity can be you know calculated, you know based on this, you know, new R value within integral of 0 to you know R radius they are here.

This total radius is some that, it will be to this R. So, at this radius what should be the average velocity that you have to calculate. Now, you have to use this trapezoidal rule and Simpsons rule. Now, how to solve this. Now, to find out that average velocity.

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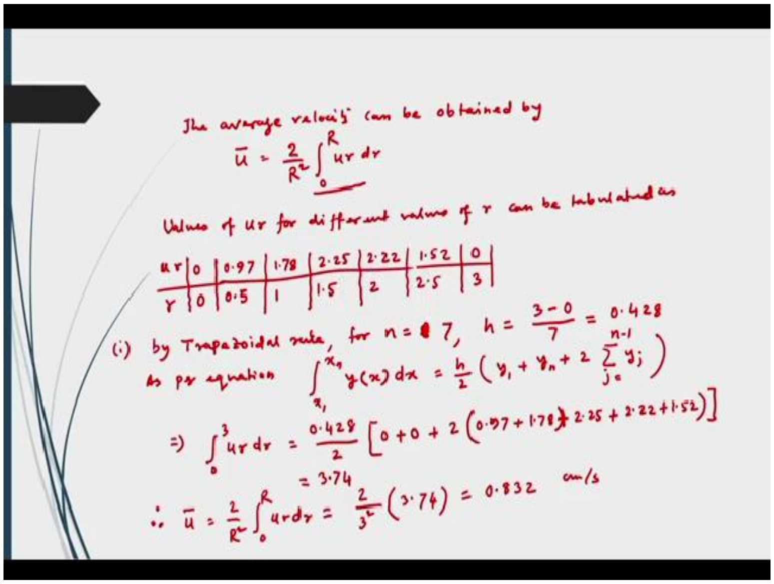

This average velocity actually given by the average here is velocity can be obtained by your means, here U bar that will be is equal to 2 by R square into 0 to R that is u r. So, based on this formula you can calculate what should be the average velocity, within this you know radius that is 0 to R are despite. Now, for this you will see now, you have to then find out first what will be the integral of the 0 to R ur dr.

Based on that, you know tabulated data given, now values of ur for the different values of R2 first calculated. So values of ur for different values of r can be tabulated as here like this first point of that is r, what should be the ur, this is ur and r first values of r r=0 then ur will be able is equal to of course 0. Second point is given 0.5 r 0.5 r value and velocity is given here. Velocity is given there according to that what should be the ur value it is coming 0.97 whereas this at r = 1 that ur will be is equal to 1.78 at r = 1.5 this you know that ur will be is equal to 2.25.

And at r = 2 this you know ur will be is equal to 2.22 and at 2.5 this ur will be is equal to 1.52 whereas, r = here 3 that ur will be is equal to again 0. Now, based on this data you have to apply what should be the you know integrals based on that, you know trapezoidal rule and then what should be the average velocity. Now applying by trapezoidal rule we can write for n = 6 here total number of point is here no it is n = 7 1 2 3 4 5 6 7.

So n = 7 here, data point and h h will be equal to r final that is 3 - initial is 0, divided by number of points here 7. So, it will be simply 0.428 and then we can write as per equation we can write x 1 to x n y x dx that will be is equal to h by 2 into y 1 + y n + 2 into summation of j = you are up to you know n - 1, j is equal to here to 2 n - 1. So, it will be is equal to here y j like this.

And then we can substitute here as like this here 0 to 3 ur dr that will be is equal to 0.428 divided by 2 here y 1 is 0 + y n is 0 and then + 2 into remaining is 0.97 + 1.78 and then plus, this is + 2.25 and then + 2.22 and then + 1.5 these are the remaining points. Then we can close this bracket here, and then finally to becoming as 3.74. Therefore hour is velocity u = 2 by r square 0 to r ur dr that will is equal to 2 by here r is given 3 then 3 square into then this integral value is 3.74.

So, finally to be coming as 0.832, this will be centimeter per second as per problem. So, in this way, we can calculate this, you know average velocity based on trapezoidal rule. Similarly, for you know average velocity if we apply the Simpsons rule what we can write here.

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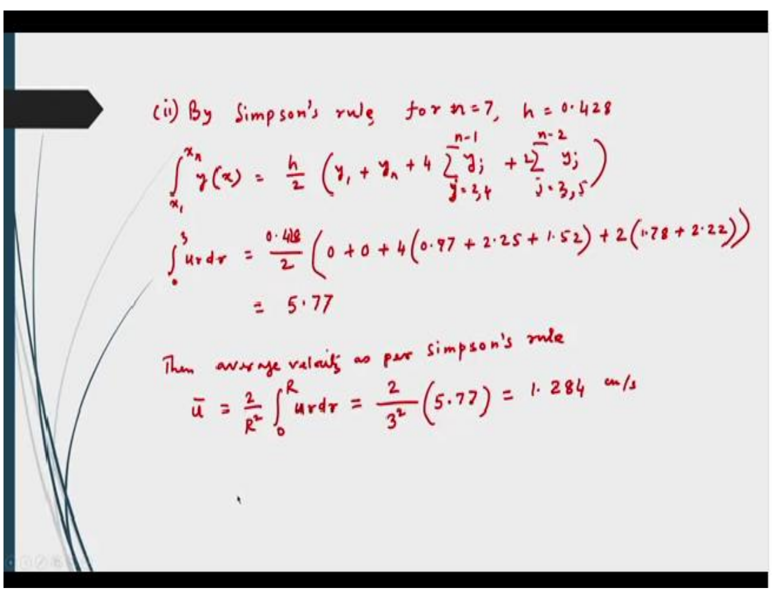

So, we can write here by Simpsons rule. By Simpsons rule here for n = 7 h = 0.428 and here x 1 to x n to y into x that will be is equal to h by 2 here it will be coming y 1 = y n + 4 summation of j here up to n - 1 j = 2, 4 and then y j + 2 into summation j = 3, 5, up to then n - 2 and then y j. So, based on this we can write here 0 to 3 ur dr. According to the tabulated data you have 0.428 divided by 2, here y 1 is 0 + y n 0 + here 4 into this up to n - 1 data to be 0.97 and then + 2.25 + 1.52.

This is your remaining data and then other parts of this data we can write as per equation of Simpsons rule n 2 into 1.78 + 2.22. So finally to becoming as 5.77 and then average velocity as per Simpsons rule can be written as you bar that will be is equal to 2 by r square integrate 0 to r, ur dr, so it will be coming as 2 y r is given to you that is 3 square into this integral value is 5.77, then finally it will be coming as 1.284 is a centimeter per second as per problem.

So, based on the Simpsons rule you can estimate what is the average velocity based on the velocity versus radial position of despite data. So, we have learned here how to calculate that you know integral values are based on that you know numerical integration proceed ur of trapezoidal rule and Simpsons on third rule or Simpsons rule simply and you can also have practice other you notability data, or you can find out that differently, you know that variables of chemical engineering processes like here 1 problems.

It is given if water is flowing to the 5 what should be the average velocity whenever it will be flowing to the 5 that can be calculated based on this integral value, but this integral value cannot be you know obtained, you know analytically because there is no certain you know equation that is represented by that you know average velocity. Even if you know that you know integral or you can see that particular function then you can easily calculate that integral value by analytical method.

But somewhere you will see that some integral or some equation will be so complicated that you may not had that you know analytical solution of that integration. So, for that you can apply this Simpsons rule or trapezoidal rule directly according to that you know that is equation and also that integral values based on that function.

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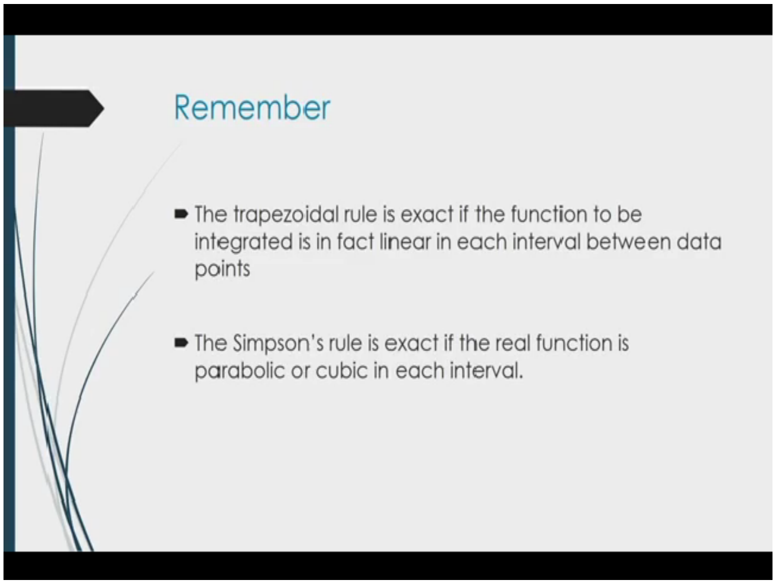

So, in this case, we have learned this trapezoidal rule and Simpsons rule. Now, the trapezoidal rule is that if the function to be integrated is in effect linear is interval between data points and Simpsons rule is exact if the real function is parabolic or cubic in each intervals. Even you can get these integrals if your function is not exactly that parabolic with some other complex you know nonlinear function there.

You can get that integral value of that nonlinear function based on this Simpsons rule. In the next lecture will try to discuss about the analysis of process degrees of freedom. So, we are here you know stopping that, you know, computational techniques, because these things is very important, this is the basic understanding of this, you know computational techniques, because you have to know that these 2 square meter to feed that you know linear equation.

And in many you know chemical engineering process even other engineering processes sometimes the experimental data to be predicted by performing an equation that is linear equation or nonlinear equation whatever it is and that nonlinear equation will have some you know parameters and that parameters can be obtained just by fitting with the experimental data. So, that can be obtained by least square method.

Even for nonlinear equation, you can simply use that you know Newton's method and also for integral values that you can use the Simpsons rule and trapezoidal rule, so it will be helpful for your further understanding of the you know process and also that variables how to calculate based on that linear and nonlinear equation and also how to feed that linear or nonlinear equation based on that experimental data.

In the next module will try to you know discuss more about that chemical engineer process and based on that process, how to analyze the degrees of freedom based on that variables, how many variables will be there with that variables how many equations will be performed and those equations whether will be you know, giving the unique solution or not that can be you know access by the degrees of freedom. So, it will be discussed in the you know next module in the next lecture. So, thank you for your giving attention.