Computational Techniques
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Module No. # 06
Differentiation and Integration
Lecture No. # 04

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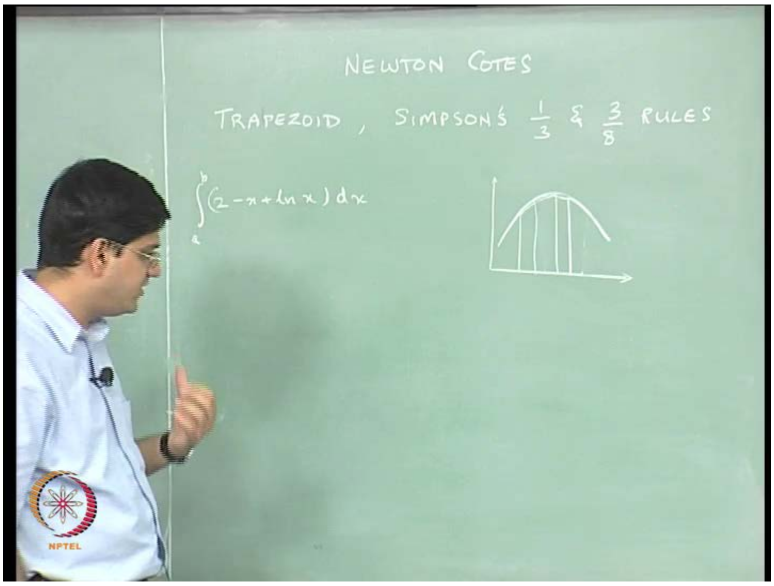

Hi, and welcome to this fourth lecture of the module on differentiation, and integration. In the previous lecture, what we were doing is we derived some of the integration formulae, these integration formulae were classified as Newton cotes integration methods, and examples of Newton cotes integration formulae. The first one was the trapezoidal method, Simpson's one-third rule, and Simpson's three-eighth rule. (No audio from 00:50 to 00:55) What I will do today is derive the error equation for the Simpson's one-third rule.

After going over the derivation for trapezoidal rule, Simpson's one-third and three-eighth rule, what we did was used Microsoft excel to find integral from a to b, I think we did it from one to two, if I am not mistaken of 2 minus x plus l n x dx that integration we did, and we used basically the trapezoidal method, the Simpson’s one-third rule, and the Simpson’s three-eighth rule. And we saw that when we use trapezoidal method with our h equal to 1 at that time there were significant errors between the actual integral value, and the numerical integral value, then when we choose h equal to 0.2; that means, we split down the overall interval.

So, this is what we wanted to find out this particular integral or I believe the integ might might have the other line might have actually been closer to that (No audio from 02:06 to 02:11) So, we wanted to find this particular integral, what we did was first applied the trapezoidal rule directly to this integral then we broke down this particular to this interval then we broke down that interval into two intervals. And then we applied trapezoidal rule and then we compare their results of the trapezoidal rule with the application of Simpson’s one-third rule. And we saw that two applications of trapezoidal rule gives less accurate results than Simpson’s one application of Simpson’s one-third rule. Although the number of intervals that trape trapezoidal rule uses and Simpson’s one-third rule uses are the same, when we are going to break down the interval the integration into two intervals for trapezoidal rules.

Next, what we did was we broke down the same in instead of two intervals; we broke it down into three intervals (No audio from 03:04 to 03:13) and found out the numerical approximation of the integration using the trapezoidal rules applying trapezoidal rules three times. Once for this interval second and third time for this interval h being 0.333 then we applied Simpson’s three-eighth rule for a single application of the three-eighth rule, which uses the point y 1, y 2, y x 1, x 2, x 3 and x 4. And we saw again that the Simpson’s three-eighth rule results were more accurate than the trapezoidal rule. And were indeed more accurate than the Simpson’s one-third rule, but the difference between Simpson’s three-eighth rule and the Simpson’s one-third rule accuracy was not that significant.

We will take another example in today's lecture more chemical engineering example, if you will will take that example to demonstrate once again, how one would use the trapezoidal or the Simpson’s one-third rule. Before doing that, I will again derive the error equation for the Simpson’s one-third rule in orde in order to show, what how the Simpson’s why the Simpson’s one-third rule is actually fairly popular.

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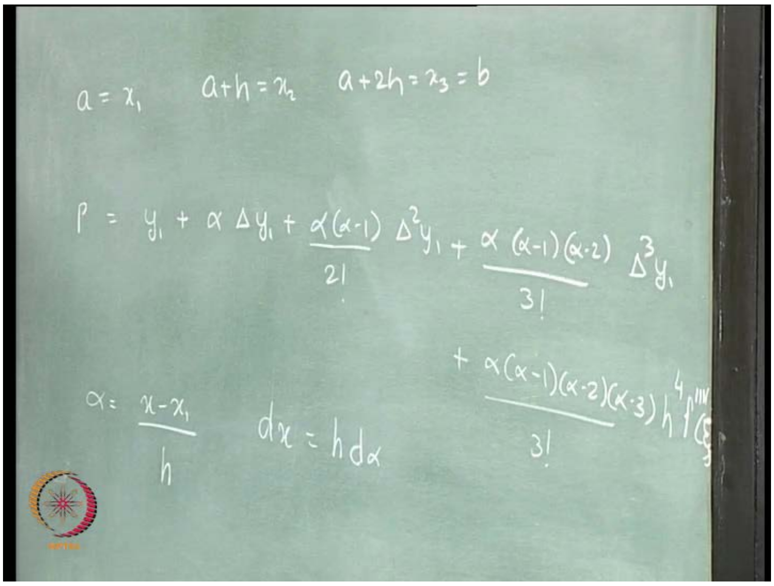

So, the polynomial that we are going to fit in Simpson's one-third rule, what what we said we are going to do is between the value a we will call that as x 1 a plus h will be x 2, a plus 2 h will be our x 3 which is our b. So, this is what we said, we are we are going to do. So, we are going to fit a polynomial to this this data and then we are going to integrate the polynomial that we fit. Now, if we were to not stop at a plus 2 h, but go ahead a plus 3 h, a plus 4 h, and so on and so forth, we will get a higher order polynomial.

So, a general polynomial p is going to be using the forward difference formula is going to be y 0 y 1 sorry plus alpa alpha times delta y 1 plus alpha square sorry not alpha square alpha alpha minus 1 by delta squared y 1 divided by 2 factorial plus alpha alpha minus 1 alpha minus 2 divided by 3 factorial delta cube y 1 plus alpha alpha minus 1 alpha minus 2 alpha minus 3 by 4 factorial into delta cube y 1 and so on.

So, this is what our polynomial is going to be, if what what we did in the previous lecture is, we said that since the polynomial is only going to be fitted to this three data points will just retain these three terms and the terms that we are neglecting are the term are the terms over here. So, because we are neglecting all these these terms there will be certain error that is going to be associated with neglecting those terms. And then we try to find out, what that error is going to be so on and so forth that is what we essentially that part of it we did not do, what we did was only retain this particular term what I am going to show today is that in the Newton's one-third rule. In fact, this term also disappears, when we actually do the integration and the leading term that that gets left is this term. This term is h to the power four accurate. So, when you integrated it will get Newton's one-third rule as h to the power five accurate.

So, the Simpson's rule, if you recall from the previous lecture was h cubed accurate where as the one-third rule is going to be h to the power five accurate rather than h to the power four accurate. And that is going to be a very important property of these Newton cotes formulae that make that makes Simpson's one-third rule actually more popular than the Simpson's three-eighth rule. So, because people have done this derivation and we know, what to expect that is why I am actually going to retain this particular term and essentially going to replace this term with the numerical with the mean value theorem. And that term, when we replace with mean value theorem is going to be alpha alpha minus 1 alpha minus 2 alpha minus 3 by 3 factorial multiplied by h to the power 4 f four dash of zeta, where zeta is some point that lies between a and a plus 4 h.

So, that is that is what will get and where alpha if if you recall is defined as x minus x 1 divided by h. So, that is the definition of alpha and therefore, the definition of there therefore, when we differentiate this equation we will get dx is equal to h d alpha. Again this is something this is something that we have done in the previous lecture is not something that that is new in this particular lecture, what we are actually going to do is see what happens, when we apply the same methodology to the Simpson's one-third rule.

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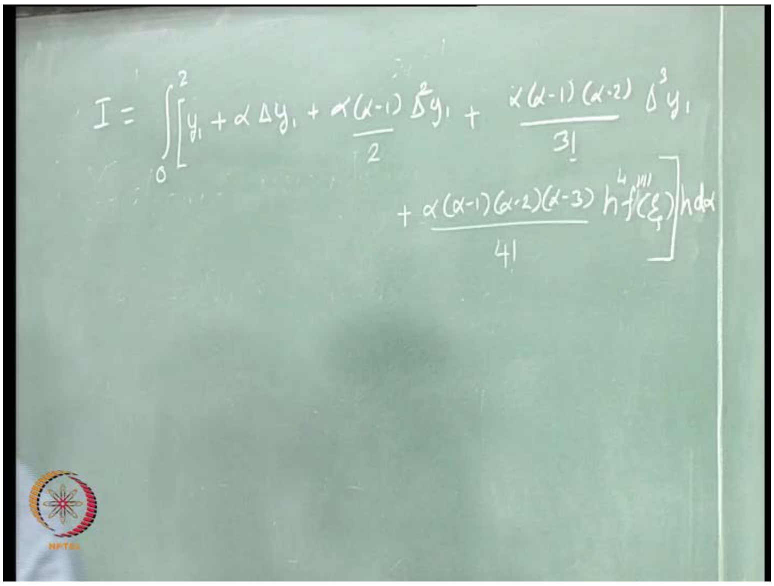

So, our I, integral I, the numerical integral I is going to be integral from x 1 to x 3, which is h equal to 0 to h equal to 2 0 to 2 y 1 plus alpha delta y 1 plus alpha alpha minus 1 delta squared y 1 by 2 plus alpha alpha minus 1 alpha minus 2 by 3 factorial delta cube y 1 plus alpha alpha minus 1 alpha minus 2 alpha minus 3 by 4 factorial h to the power 4 f four dash. I will just write it a little rewrite this. So, the next term after this is going to be plus alpha alpha minus 1 alpha minus 2 alpha minus 3 by 4 factorial h to the power 4 multiplied by f four dash of y sorry f four dash of zeta that is our polynomial that, we had over here. I have written that polynomial and integral of that polynomial with dx is what our I is and dx is h d alpha.

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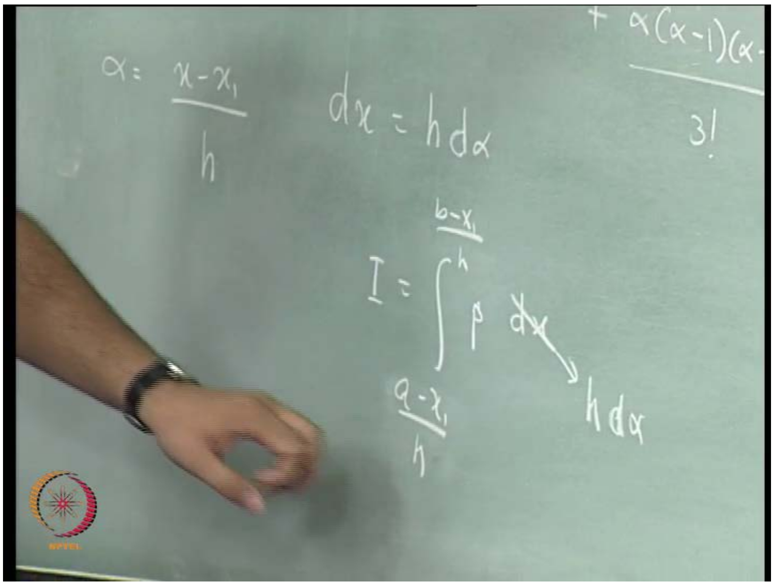

So, our dx was h d alpha remember, what we want to do our I is nothing but integral from x minus a divided by h are sorry a minus minus x 1 divided by h to b minus x 1 divided by h p dx and dx is going to be replaced by h d alpha. So, we have, where a is nothing but our x 1 so, this is zero b is a plus 2 h. So, that is a plus 2 h minus a, which is divided by h which is two so that is why, we get zero to two p multiplied by h d alpha again this this is something that we have done in the previous lecture.

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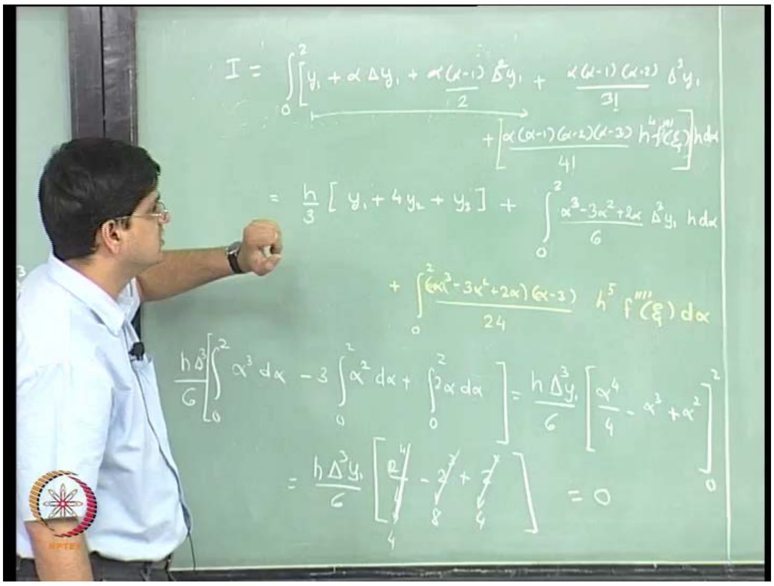

In the previous lecture, we had considered all these terms and based on these terms. We had obtain the integral of i, the integral i using the Simpson's 1 3rd rule and that particular result essentially gave us h divided by 3 y 1 plus 4 y 2 plus y 3 that was the result that we derived in the previous lecture. Now, talking about this particular guy we have integral from 0 to 2 this is alpha squared minus 2 alpha sorry minus 3 alpha plus 2 so, that is multiplied by alpha. So, alpha cube minus 3 times alpha squared plus 2 times alpha divided by 6 which is 3 factorial multiplied by delta cubed y 1 h d alpha is this particular guy. And this final term, over here is going to be we will we will write that as integral from 0 to 2 this is alpha multiplied by alpha square minus three l this is going to be alpha cube minus 3 alpha squared plus 2 alpha multiplied by alpha minus 3 divided by 24 and it will h to the power 5 f four dash zeta times d alpha.

Now, we will just consider the term this particular term and do the integration and when we do that, we will we will get integral from 0 to 2. One we will have basically delta cubed h delta cube by 6 outside the integral sign and we will have inside integral it is going to be alpha cubed d alpha minus 3 times integral alpha squared d alpha plus integral from 0 to 2 alpha d alpha or actually 2 alpha d alpha sorry. This is what, we will get that we will be able to write as h delta cubed y 1 by 6. This is going to be alpha to the power 4 divided by 4 minus 3 alpha cube divided by 3 which is just going to be alpha cubed plus 2 alpha squared divided by 2, which is just alpha squared going from 0 to 2 which we will be able to write as h delta cubed y 1 divided by 6 multiplied by alpha alpha to the power 4 divided by 4 which is 2 to the power 4 that 16 by 4 that is 4 minus 0. So, it is 2 to the power 4 by 4 minus alpha cubed which is 2 to the power 2 sorry 2 to the power 3 plus 2 squared. So, this is 16 divided by 4 which is 4 this is 8 and this guy is 4. So, here what we have is 4 minus 8 plus 4 that is 8 minus 8 that is 0. So, this particular term has become 0.

So, what has happened is, when we retain an additional term in this integration, when we actually do the integration and substitute the values of the limits of integration into this particular equation, what we realize is that after integration this term drops out. So, the error is not going to be governed by this particular term, but in order to figure out the error. We have to include and additional term over here and that particular additional term is essentially this term. And then we go ahead and do the integration of this term to indeed see that after doing the integration that particular term does not disappear.

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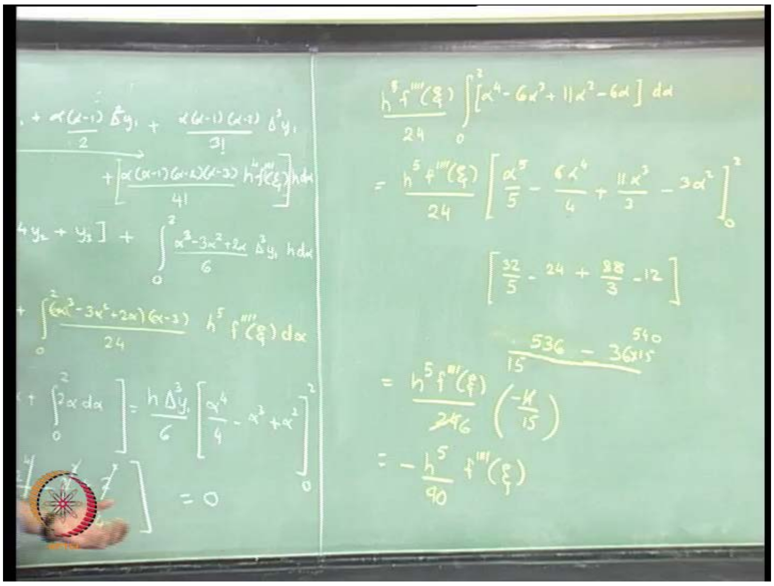

So, what we will write is h to the power 5 f four dash of zeta divided by 24 multiplied by integral from 0 to 2 we have essentially alpha to the power 4 minus 3 alpha cubed plus 2 alpha squared minus 3 alpha cubed minus plus 9 alpha squared minus 6 alpha (No audio from 17:19 to 17:25) d alpha. So, 3 minus 3 alpha cubed minus 3 alpha cubed is going to be minus 6 alpha cubed. I will write down over here and plus 2 alpha squared plus 9 alpha squared is going to be plus 11 alpha squared minus 6 alpha d alpha, which is going to be equal to h to the power 5 (No audio from 18:01 to 18:07) 24 divided by 24 alpha to the power 5 divided by 5 minus 6 alpha to the power 4 divided by 4 plus 11 alpha cubed by 3 minus 3 alpha squared from 0 to 2.

So, this guy is going to be 32 minus 0 divided by 5. So, it is 32 by 5 minus 6 alpha to the power 4 by 4 alpha to the power 4 is 16 16 divided by 4 is 4 4 multiplied by 6 is 24. So, minus 24 plus 11 by 3 alpha cubed. So, that is going to be 88 by 3 and minus 3 times 4 is minus 12. So, this is 32 three 96 by 5 plus 88 multiplied by 5 eight fives are forty and eight times five is forty 440 divided by 15 minus 36 36. So, these is going to be five thirty six this guy 536 by 15 minus 36 and are it is going to be minus 36 multiplied by 15. So, fifteen six times six is ninety zero nine carried over forty five fifty four. So, what we get is thirty six minus a 536 minus 540 that is minus four by fifteen.

So, we will have h to the power 5 f four dash of zeta divided by 24 multiplied by minus 4 by 15 this and we get 6 over here times fifteen time six is ninety. So, this is minus h to the power 5 divided by 90 f four dash of zeta. So, this is the error in computing the integral using the Simpson's one-third rule. So, the error in integral of Simpson's one-third rule is of the order of h to the power 5. If you recall from the previous lecture error in inte in finding the integral using the trapezoidal rule was h to the power three.

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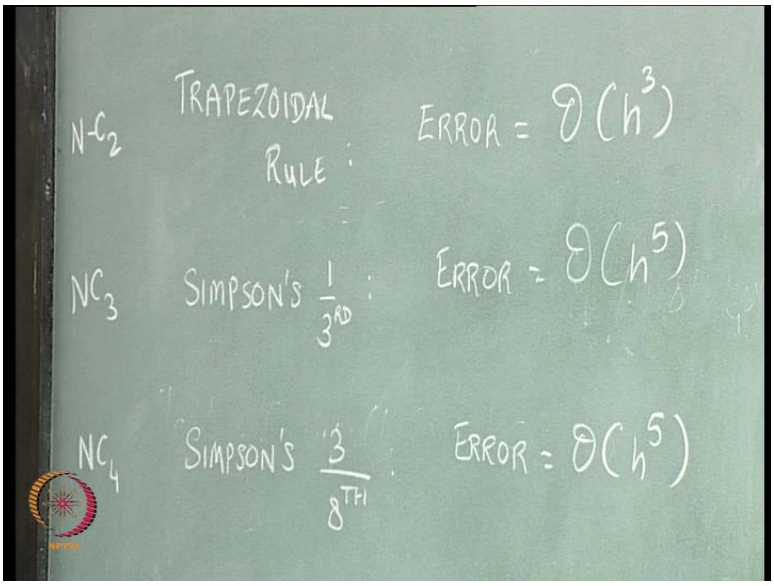

So, I will write those results now

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This is something that we have not derived yet, I am just stating it as it is that the error in case of Simpson's three-eighth rule is order of h to the power 5, what happens in Simpson's three-eighth rule is that we will use this this this and this term the four terms, we will use to derive the three-eighth rule the way we way we talked about in the previous lecture. And this particular leading term will give us an indication of whether or not the error is h to the power 5 accurate or it is even more accurate than that when we do the derivation for Simpson's three-eighth rule, we will find that this particular term does not disappear, this particular term also stage there this term is h to the power 4. We will get another h factor because of dx equal to h h d alpha. So, we will have this particular term, when we do the integration corresponding to h to the power 5 that term, because it does not drop out as a result of that term, we have the accuracy of the Simpson's three-eighth rule to be h to the power 5.

So, the trapezoidal rule is h cubed accurate, Simpson's one-third rule is h to the power 5 accurate, Simpson's three-eighth rule is again h to the power 5 accurate. This uses two intervals. So, this is I will call this NC 2 Newton cotes formulae with two intervals. Simpson's one-third, we can call NC 3. Simpson's three-eighth, we can call NC 4, what we will do is go to excel and do one chemical engineering problem of interest and problem that we will do here is going to be design of a plug flow reactor.

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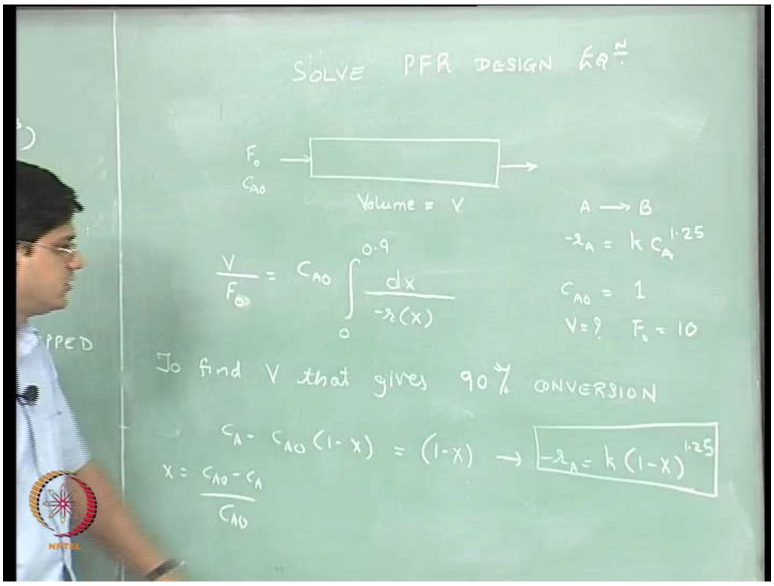

So, we will solve PFR design equation (No audio from 23:47 to 23:54) the design equation for plug flow reactor. So, what we talk about in plug flow reactor is we have the flow coming in with a velocity of F naught the overall the volumetric flow rate F naught the overall volume of PFR (No audio from 24:17 to 24:21) is going to be V. Some reaction takes place let us let us call that as A going to B that is the reaction taking place within the system and let say rate minus r A is some k times C A to the power say 1.2 or say 1.25 arbitrarily numbers.

So, this is let say the rate of reaction taking place in the PFR, we have the flow rate coming in at F 0 initial concentration of the overall the overall initial concentration of this specious let us say is C A0. So then, we the equation is F v by F 0 is going to be C A0 integral from 0 to x exit dx by minus r x, where r is really the rate rate of reaction. This is the expression that we get for doing this to find the volume of the PFR that will give a desired exit concentration.

So, let say that, we want to find (No audio from 26:49 to 26:04) we want to find the volume of the reactor that gives ninety percent conversion; that means, x at the exit is going to be ninety percent or 0.9. So, the problem that we have is V by F naught equal to C A naught dx by minus minus r A. Let us assume that C A naught we will just use some arbitrarily data C A naught is one moles per meter cubed, let us say we want to find out the volume, let us say the flow rate F naught is say ten meter cubed this is the overall data that is that is actually given to us.

The rate of reaction is r equal to k CA to the power 1.25 and CA the way it is related to the conversion is … So, conversion is C A naught minus C A divided by C A naught. So, C A is going to be C A naught multiplied by 1 minus conversion that comes essentially from definition of conversions conversion, which is C A naught minus C A divided by C A0. So, you multiply C A0 over here. So, you will get C A naught x equal to C A naught minus C A or C A equal to C A naught minus C A naught x, which is essentially this substituting the value of C A naught equal to 1. In this particular equation C A is going to be 1 minus x and therefore, r minus r A is going to be k times 1 minus x to the power 1.25. (No audio from 27:49 to 27:54)

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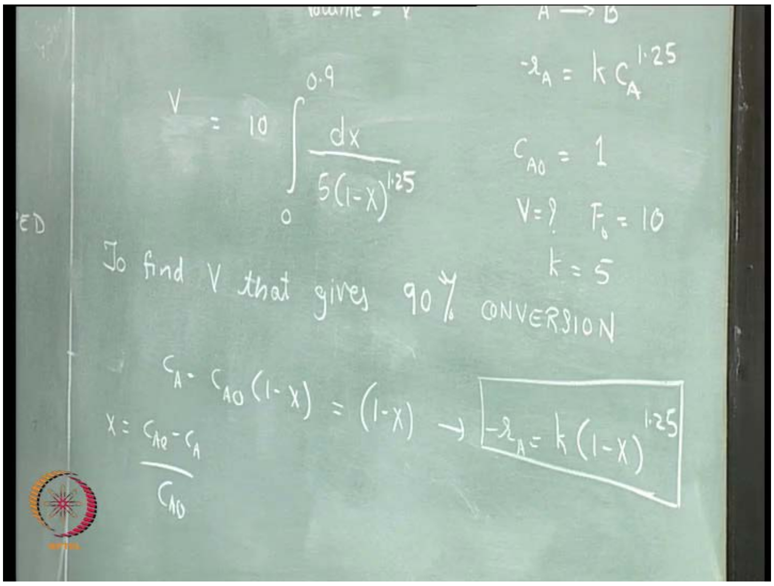

And, when we substitute this particular equation into this and we substitute all the values over here. We will get V divided by F 0, which is 10 equal to C A naught, which is 1 multiplied by d x divided by minus r A and minus r A is going to be k times 1 minus x to the power 1.25. We will take 10 on to the other side. So, we will get V equal to 10 times integral from 0 to 0.9 dx divided by k 1 minus x to the power 1.25. And let let us, arbitrarily take the value as of k as 5. So, we will substitute that value also over here as this.

So, the integral that we are interested in finding is V equal to two multiplied by integral from 0 to 0.9 dx divided by 1 minus x to the power 1.25. So, that is the problem that we are going to try to solve using various numerical integration techniques by using Microsoft excel.

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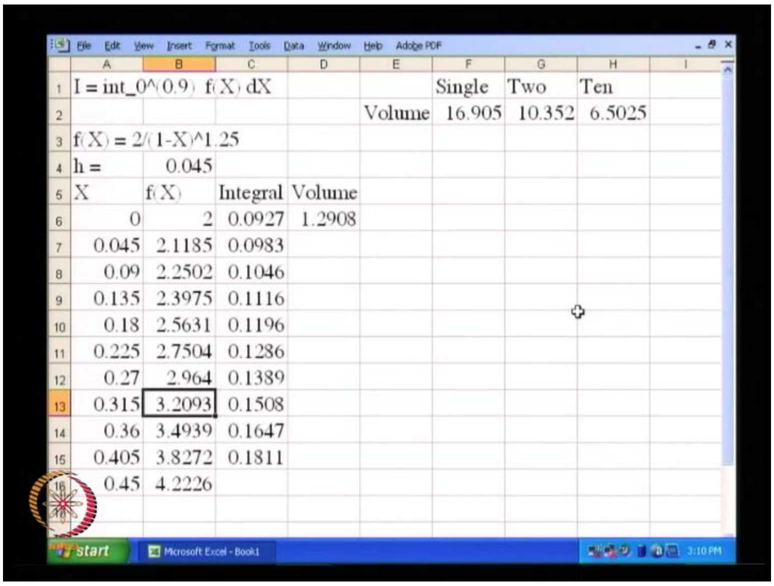

	A	B	C	D	E	F	G	H
1	I = int_0^(0.9) f(X) dX					Single	Two	Ten
2					Volume	16.905	10.352	6.5025
3	f(X) = 2/(1-X)^1.25							
4	h =	0.045						
5	X	f(X)	Integral	Volume				
6	0	2	0.0927	1.2908				
7	0.045	2.1185	0.0983					
8	0.09	2.2502	0.1046					
9	0.135	2.3975	0.1116					
10	0.18	2.5631	0.1196					
11	0.225	2.7504	0.1286					
12	0.27	2.964	0.1389					
13	0.315	3.2093	0.1508					
14	0.36	3.4939	0.1647					
15	0.405	3.8272	0.1811					
16	0.45	4.2226						

So, what we want to do is, I equal to integral from from 0 to 0.9 (No audio from 29:23 to 29:33) f of x dx that is the integral that we want to find f of x, where x is the conversion as we have written on the board f of x is going to be 1 sorry 2. So, because we get ten divided by five that gives us two divided by 1 minus x to the power 1.25 that is going to be our f of x and we want our x to go from 0 to 9. So, our integral I is nothing but the total volume. So, let us write write our write down the x value and we are going to start with x equal to 0 and we also need to decide, what our h is going to be h let say is going to be equal to 0.9.

So, our x is going to be equal to the previous value plus the h and we do f 2 and put dollar signs over there. So, that when we drag it, the value does not change then we use we compute f of x f of x is going to be equal to 2 divided by 1 minus x to the power 1.25.

And we just go and drag this. So, this is the value of f of x at x equal to 0.9 and this is the value of f of x at x equal to 2. And our volume is going to be just the final integral at at x equal to 0.9. So, using the trapezoidal rule it is going to be equal to our h divided by two that is this value, we will put the dollar signs over there divided by 2 multiplied by y 1 plus y 2 that is going to be our our integral.

So, the volume of the reactor that is required base obtain from the trapezoidal rule application of the trapezoidal rule only once is going to be 16.9. Instead of that, if we were to apply the trapezoidal rule twice, we will get a better value of of the integral. So, what I will do is volume required and I will write down the values from the trapezoidal rule then the Simpson's one-third rule and the Simpson's three-eighth rule this copy this and do paste special just copy the value over there this is h equal to 0.9 or single application, two applications and ten applications of the rules.

Now, if we were to use two applications of the rules our h is going to be 0.45 and we just have to drag it once, drag this one's, drag this. And if we do f 1, we will get the appropriate value. If if we do f 2 again, we will get this appropriate value. And our total volume is going to be equal to this plus this. (No audio from 33:32 to 33:37) So, total volume is going to be equal to this guy plus the next guy. So, the volume that we get on two applications of this of the trapezoidal rule is going to be as shown over here. (No audio from 33:52 to 33:56) 10.352

Now, let us say we want to do ten applications then we will go for h equal to 0.09. And we just copy this down ten times (No audio from 34:08 to 34:18) and then we just have to some more all of this (No audio from 34:20 to 34:27) not this not this guy and the ten applications are giving us the value of the volume that is obtained as 6.5025. So, what we are seeing over here, is as the number of applications of the trapezoidal rule or increasing the value keep decreasing let us do twenty iterations.

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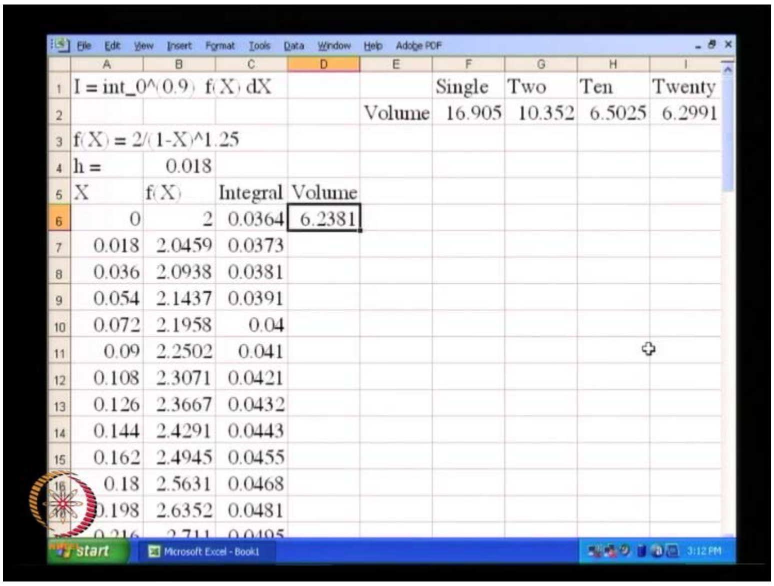

So, that is going to be equal to 0.9 divided by 20. And when we do that, we will have to just drag drag this further (No audio from 35:07 to 35:17) and we will have to this double click this double click this and this is going to be just the summation for this entire range(no audio from 35:38 to 35:43) So, as you can see that were twenty applications the value of the volume is now beginning to converge. Let us do fifty applications now and h then is going to be equal to 0.9 divided by fifty.

And we just drag this for many more cells. So, that we reach 0.9 (No audio from 36:20 to 36:31) go up and double click this go up double click this go to the last value delete the last value. And we find the volume as the sum of the entire number of intervals that we have obtained and the volume that we get is 6.238. So, what we see is that finally, it seems the method seems to be converging, what we need to do is we need to define our error value and we need to use large enough number of intervals such that this this particular method finally, converges to the final volume that we are interested in.

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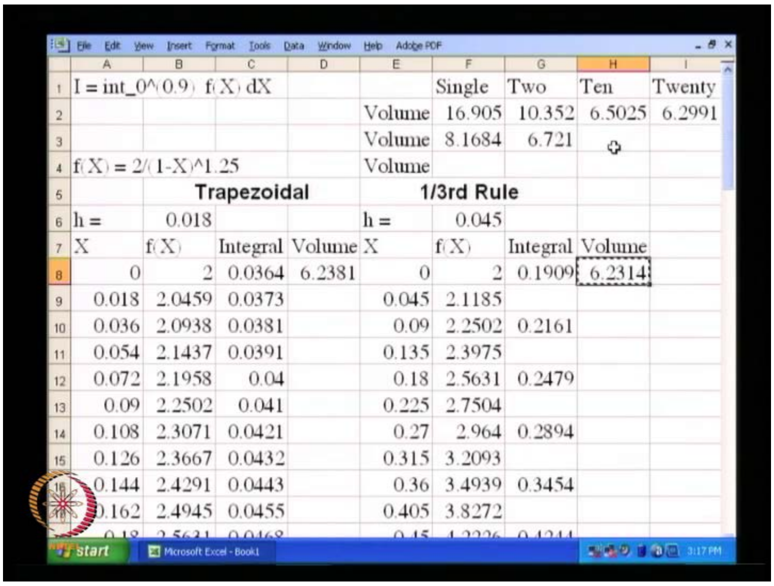

	A	B	C	D	E	F	G	H	I
1	I = int_0^(0.9) f(X) dX					Single	Two	Ten	Twenty
2					Volume	16.905	10.352	6.5025	6.2991
3					Volume	8.1684	6.721		
4	f(X) = 2/(1-X)^1.25				Volume				
5		Trapezoidal			1/3rd Rule				
6	h =	0.018			h =	0.045			
7	X	f(X)	Integral	Volume	X	f(X)	Integral	Volume	
8	0	2	0.0364	6.2381	0	2	0.1909	6.2314	
9	0.018	2.0459	0.0373		0.045	2.1185			
10	0.036	2.0938	0.0381		0.09	2.2502	0.2161		
11	0.054	2.1437	0.0391		0.135	2.3975			
12	0.072	2.1958	0.04		0.18	2.5631	0.2479		
13	0.09	2.2502	0.041		0.225	2.7504			
14	0.108	2.3071	0.0421		0.27	2.964	0.2894		
15	0.126	2.3667	0.0432		0.315	3.2093			
16	0.144	2.4291	0.0443		0.36	3.4939	0.3454		
17	0.162	2.4945	0.0455		0.405	3.8272			

It is the same idea that was used in checking the convergence of the various methods that we will use over here as well. I will just (No audio from 37:32 to 36:37) write this aligns alignment merge and center aligned and I will write this as trapezoidal method. Next, what I will do is use Simpson's one-third rule in order to get this particular to solve this same problem. (No audio from 38:02 to 38:09) And again, we will use h equal to 0.9 divided by 2. Keep in mind that in application of the one-third rule, we will have to use in application of one-third rule.

We will have to use even number of intervals in trapezoidal rule in the number of intervals did not matter. We will again have f of x sorry we will have again x f of x integral and then the total volume using the one-third rule. We will start off with 0 and as it was here, we will just copy this and then just move this guy over here. And this should be good our f x, I will just copy this, I will just move this over here.

So, the Simpson's one-third rule the integral was so, in the in the trapezoidal rule the integral was nothing but h by two multiplied by y 1 plus y 2. In this case, the integral is going to be equal to h divided by three. So, I will put the dollars because h is not changing divided by three multiplied by y 1 is this guy plus four multiplied by y 2 plus y 3 that is the integral and the volume is nothing but just this particular value.

So, the volume that we are getting from the single application of Simpson's one-third rule is 8.17 approximately. I will just paste it over here. Now, two applications of the

Simpson’s one-third rule means once we will applied from 0 to 0.45 and the second time we will apply from 0.45 to 0.9. So, we are going to divide this by four this time and we will apply this. And then integral again we have to compute between 0.45 and 0.9 right. So, what we need to do is y 1 plus 4 y 2 plus y 3 multiplied by h by three. So, this is what we need to do and the volume that is to be computed is going to be this entire sum over here.

So, two applications of Simpson’s one-third rule give us a volume of 6.71. And ten applications, we will have to divide this by twenty. So, the ten applications will actually give us (No audio from 41:21 to 41:29) Let us to see, what will get, (No audio from 41:31 to 41:47) I will just keep pasting. (No audio from 41:48 to 41:59) So, this is going to be y 1 plus 2 y 4 y 2 plus y 3 multiplied by h by three this is all going to use then these three points this will use these three points so, on and so forth. And the volume is going to be the entire sum that we just need to go and drag it over here and the volume that we get is 6.23 using ten applications.

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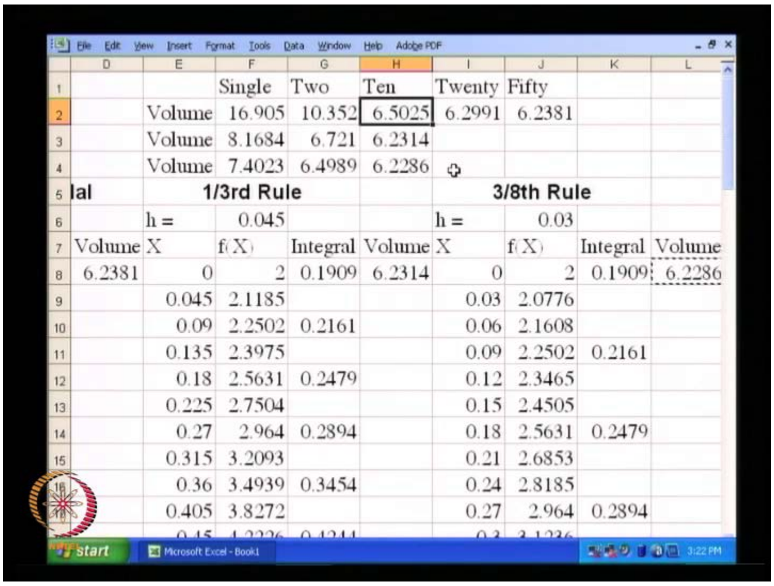

	D	E	F	G	H	I	J	K	L
1			Single	Two	Ten	Twenty	Fifty		
2		Volume	16.905	10.352	6.5025	6.2991	6.2381		
3		Volume	8.1684	6.721	6.2314				
4		Volume	7.4023	6.4989	6.2286				
5	lal	1/3rd Rule				3/8th Rule			
6		h =	0.045			h =	0.03		
7	Volume	X	f(X)	Integral	Volume	X	f(X)	Integral	Volume
8	6.2381	0	2	0.1909	6.2314	0	2	0.1909	6.2286
9		0.045	2.1185			0.03	2.0776		
10		0.09	2.2502	0.2161		0.06	2.1608		
11		0.135	2.3975			0.09	2.2502	0.2161	
12		0.18	2.5631	0.2479		0.12	2.3465		
13		0.225	2.7504			0.15	2.4505		
14		0.27	2.964	0.2894		0.18	2.5631	0.2479	
15		0.315	3.2093			0.21	2.6853		
16		0.36	3.4939	0.3454		0.24	2.8185		
		0.405	3.8272			0.27	2.964	0.2894	

This is already quite close to the fifty applications of the trapezoidal rule. So, just ten applications of the Simpson’s one-third rule are going to be going to come very close to thirty applications of fifty applications of the Simpson’s of the trapezoidal rule. And we will just go and solve this for the Simpson’s three-eighth rule. And in three-eighth rule the h has to be the single application for single application h has to be equal to one-third of the the total value. And we we will just be able to copy these guys over here for the three-eighth rule, we will just increase the size (No audio from 43:48 to 43:49) and integral has to be equal to the h that we use is going to be here.

So, x will be x 0 plus this h and we will just drag this over here f 2 this is correct, we will just drag this integral is going to be three multiplied by multiplied by h divided by eight multiplied by y 1 plus 3 y 2 plus 3 times y 3 plus y 4. And the volume is just going to be equal to the integral for this particular case. We just copy this volume and paste it over here and now, we do two applications of the Simpson's three-eighth rule the two applications of the Simpson's three-eighth rule (No audio from 44:57 to 45:04) will lead as to the volume equal to six point almost 6.5.

And for ten applications of Simpson's three-eighth rule, we just have to use h equal to 0.03 (No audio from 45:24 to 45:37) I just drag this and then copy we have to skip to cells and paste one, two cells has skipped and then paste, one, two cells has skipped and then paste again. And these values we do not need and this guy is going to be sum of this entire structure. And as you can see with that with ten applications the volume that we get is approximately 6.23.

So, this is the volume that we will get with single application of the trapezoidal rule, two applications of the trapezoidal rule even with ten applications of the trapezoidal rule. We find at the actual value is fairly far away from the the value of they they actual volume that will be needed. So, we actually need to go to fifty or may be or seventy applications of the Simpson's of the trapezoidal rule in order to get the actual value whereas, it with respect to the Simpson's one-third rule will perhaps need about twenty applications and with the Simpson's are may be twenty five applications for the Simpson's three-eighth rule, we will perhaps need something like fifteen applications. Fifteen applications of the Simpson's three-eighth rule require about forty five data points whereas, twenty applications of the Simpson's one-third rule one-third rule require forty data points.

So, that is the amount of effort, how the overall effort in this particular case scales. So, to recap what we have done so far is we have considered the trapezoidal rule, Simpson's one-third rule and the Simpson's three-eighth rule did the derivation of the trapezoidal rule using multiple methods. The first method that we use was a geometric method. The second method that we use was fitting a straight line to the data to the data points. And the third method that we use was using the Newton's forward difference formula then we expanded the Newton's forward difference formula to take care of Simpson's one-third and the three-eighth rule.

Then we considered a simple example of f of x equal to two minus x plus l n x integral from 1 to 2 of that particular expression. And we compared Simpson's one-third, three-eighth and the trapezoidal rule using that method. And today, what we have done is shown that the errors in the one-third rule scale very nicely compared to the the trapezoidal rule. A specifically the errors in the Simpson's one-third rule are h to the power five order of magnitude whereas, for the one-third rule is sorry for the trapezoidal rule is h to the power three order of magnitude.

And then finally, we took a chemical engineering example a real life example of interest towards as chemical engineers. And showed where the numerical integration can be actually applied, what we have done finally to figure out, how many intervals are needed is, what is known as some kind of a grid independent steps, what we need to do with respect to any numerical method any integration or o d e solving method that we that we are going to use is use a number of intervals and go to a large of intervals. So, that the results do not change by changing the number of intervals any further.

As we saw in the one-third rule going from ten intervals to twenty intervals still improve the volume that we get using this the Simpson's rules. As a result of this we we have to use a large number of large number of iterations and just to finish off. I will just go once again to the board and show you why exactly we require a large number of iterations in this particular example that we have taken to finish of this example.

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So, our f of x was two divided by 1 minus x to the power 1.25 2 divided by 1 minus x to the power 1.25. If we plot this particular curve of going from x equal to 0 to x equal to 0.9 at x equal to 0 this value is approximately equal to two not approximately at x equal to 0 this value is exactly equal to 2 and at x equal to one this particular value is essentially going to be infinity. So, the the curve the way the curve look is going to be somewhat like this, what we are interested in when we say we want to find the volume of the PFR, what we are interested in doing is to find the area under the curve going from x equal to 0 to x equal 0.9. This is the curve that we interested in this is the area that we are interested in…

When we use a single application of the trapezoidal rule, I will show that with a yellow color chalk, when we use a single application of the trapezoidal rule, we are connecting these these two points with this yellow line and we are approximating this integral as the this particular area. As a result there are significant errors with that we get using the trapezoidal rule. Now, two applications of trapezoidal rule mean that, we consider a data point 0.45 at 0.45 which is essentially this guy. So, two applications of trapezoidal rule are going to be area under this the new yellow curve.

So, this is going to be the area that we will get as the numerical approximation of the the actual volume using the trapezoidal rule and so. This area under this yellow curve there are significant errors associated with it again. As a result, when we had two implementation of the trap two implementations of the trapezoidal rule there were significant errors.

Now, when we are going to use the Simpson's one-third rule, what we are doing is we are trying to pass a second order curve through these three points a second order curve through this these three points may may perhaps look somewhat like like this. So, it is again it is not following the height curve perfectly, but perhaps it will do a better job or not perhaps usually it will definitely do a better job than connecting just three the three of these data points with straight lines. As a result the yellow area that I am showing as hatched line with a single application of the trapezoidal sorry single applications of the Simpson's one-third rule that itself is significantly better than two applications of the one-third rule of the trapezoidal rule.

So, that is the reason, why we get significantly better performance, when we apply that is the geometric interpretation, why we get the significantly better performance, when we apply the one-third rule rather than two applications of the trapezoidal rule. And numerically speaking, why we get such a better behavior is that the trapezoidal rule is order of h to the power 3 accurate. And the one-third rule is order of h to the power 5 accurate.

So, this is where we finish this particular lecture in this module the forth lecture in module six. In the next lecture, we will cover one more interesting method, and one more way of actually deriving the integration formula for the trapezoidal rule; that is what we will cover. In the next lecture, and finish of this particular module in the next lecture, Thanks.