Computational Techniques.
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Module No. # 09

Lecture No. # 03

Partial Differential Equations

Welcome to lecture three of module of number 9. In this module, we are discussing numerical methods to solve partial differential equations. What we have done in the previous lecture is introduce a couple of examples for partial differential equations of the various types, like the one was the hyperbolic type of equation, parabolic and the elliptic type of equation. And we saw the numerical methods in order to solve each of those types of equations.

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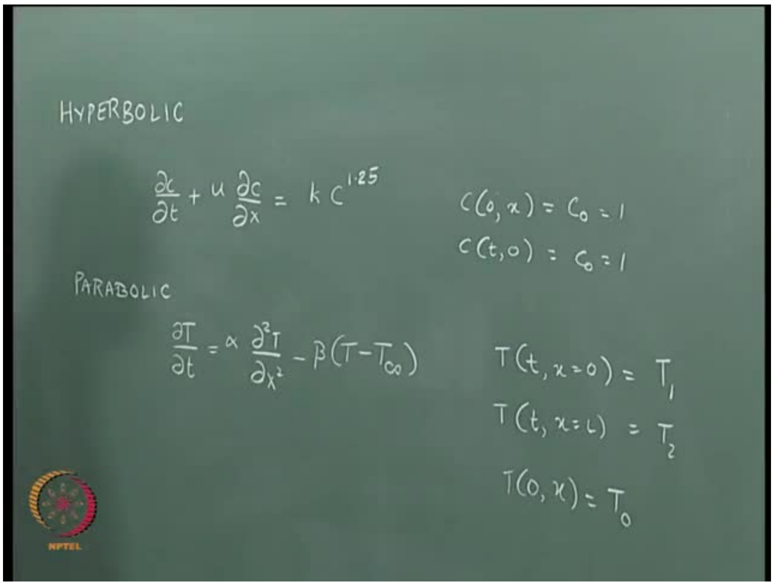

So, the examples, we are going to take in today's lecture are essentially going to be example of, one example of a parabolic equation and another example of a hyperbolic equation. So, for hyperbolic equation, we will take transient heat transfer through a rod. Sorry, for a hyperbolic equation, will take transient plug flow reactor equation and thaT is going to be d c by d t plus u d c by d x, equal to k multiplied by c to the power 1.25, starting with c at time zero and at all locations is going to be equal to some value c zero and that c zero we have taken as 1; c at all times and at location x equal to zero is also going to be equal to c zero. Then we are going to track how as the reaction takes place how the concentration c changes both with location and with time.

So, thaT is going to be the example of hyperbolic equations that we are going to use and the example of parabolic equation, this will be the heat transfer through a rod, the transient heat transfer through a rod example, and there we have partial T by partial t, is going to be equal to alpha partial square T by partial x square minus beta T minus T infinity. For simplicity, we will use the dirichlet type of boundary conditions instead of neumann type boundary conditions. That is going to be, the temperature at all times at x equal to zero is going to be some T 1, let us call that, and temperature at all times at x equal to l, we will call this as some temperature T 2.

This is going to be our parabolic equation and of course, we also need initial condition in time and T at time equal to zero and all x is given as some temperature, T zero. So, these are the two examples that we are going to solve. We will start off with the parabolic equation example and for the parabolic equation, one of the methods, we said that we can use is finite difference method in which we will use the forward in time central in space methods.

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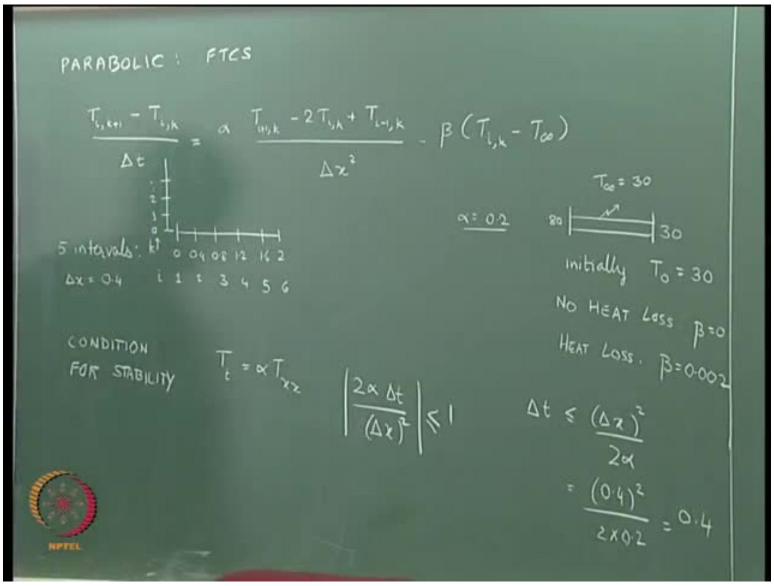

So, forward in time central in space is going to be, for parabolic, the FTCS method is T i comma k plus one minus T i comma k, divided by delta T is going to be equal to alpha multiplied by T i comma, sorry T i plus one comma k, minus two T i comma k, plus T i minus one comma k divided by delta x squared minus beta times T i comma k minus T infinity.

Now, initially what we will do is we will solve this particular problem, assuming that beta equal to zero and then we will take up a problem in which we will take a finite value of beta. So, the problem that we are going to solve initially is that there is a rod and that rod is kept. Initially, the rod is cold at room temperature. And all the ambient thaT is T infinity is going to be at 30 degrees also. This end, we will say is kept at 80 degrees. This end is kept at 30 degrees and we will solve two problems, firsT in which there is the heat loss taking place from the rod to the surrounding. Actually, that we will solve later, but first we will solve the problem where there is no heat loss taking place from the rod to the surroundings.

If there is no heat loss; for no heat loss, beta is going to be equal to zero. If there is heat loss, then let us take beta equal to 0.002 second inverse. That is going to be the units for this beta that we are to take. Alpha value, we will take it alpha, so for steel for example, alpha is going to be appropriately 0.2 centimeter square per second. So, this is the value of alpha that we will take in this particular example and let us take the length of this rod as two centimeters. So, we have this entire rod length going from zero to two, and we want to find out the temperature, how the temperature varies, with respect to time and with respect to space.

So, let us divide this particular region into n intervals and n we will take in this particular case as 5. So, we will have five intervals. So, our delta x is going to be equal to 2 divided by 5 and that is basically going to be equal to 0.4, 0.8, 1.2, 1.6 and 2. The location i index will go from 1, 2,3,4,5 and 6. Then this is going to be in the x direction and likewise in the z in the t direction, we will have various delta t's and this is of the k that i will write k will be zero, k will be one, k will be two, and so on and so forth. So, this is what we are we are going to do and the condition for stability and again we are not going to prove this but…. (no audio between: 07:41-07:52)

So, if we have the original equation as T t equal to alpha T x x that means we have, if we go to this equation (Refer Slide Time: 08:05) and if we are just going to look at this particular part, the homogeneous part of this equation, if this is going to be our overall equation, the condition for stability is going to be two alpha multiplied by delta t divided by delta x squared and should be less than or equal to one. If this condition is met, our overall scheme is going to be stable and if this condition is not met, our scheme is going to be unstable.

To puT iT in another way, iT is going to be delta t should be less than or equal to delta x square by two alpha and delta x square by two alpha is going to be equal to 0.4 square divided by two alpha and alpha value, we took as 0.2, so divided by two multiplied by 0.2. So, our delta t has to be less than or equal to 0.4. So, what we are going to do is we are going to take several different values of delta t for the value of delta x taken to be equal to 0.4, for value of alpha equal to 0.2 of value of beta equal to zero.

So, thaT is the first problem that we are going to solve. Then we will take a larger value of delta t and see what we mean by instability and the third thing then we are going to do is take our delta t under the stable conditions, solve it using Microsoft excel with the actual problem that we wanted to solve thaT is with beta equal to 0.002. Now, I will rearrange this particular equation and I will take this guy on to the right hand side. I will first multiply by delta t, take this guy on to the right hand side and rewrite that equation

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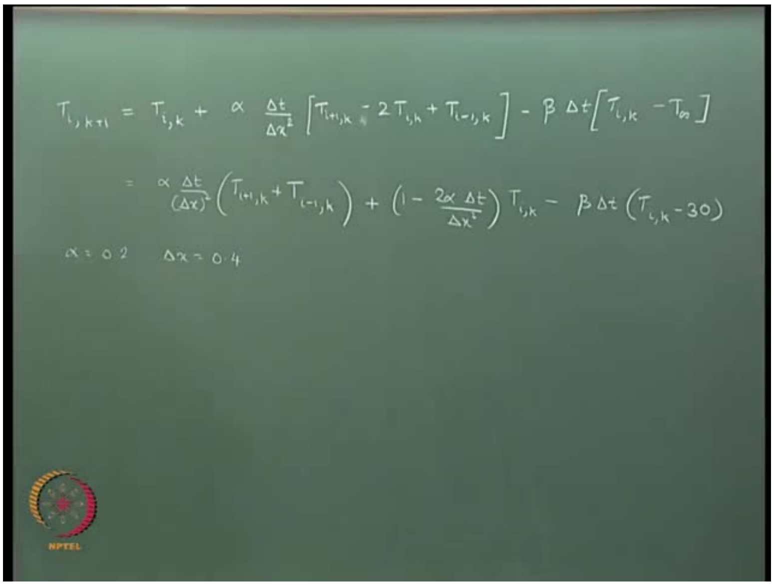

We will get that equation as T i comma k plus one should be equal to T i comma k, plus alpha delta t by delta x square, multiplied by T i plus one comma k minus two, T i comma k, plus T i plus one i T i minus one comma k, minus beta delta t multiplied by T i comma k minus T infinity. So, this we can take T i comma k along with rest of the stuff, so we can have alpha delta t by delta x square multiplied T i plus one comma k plus T i minus one comma k plus one minus two alpha delta t by delta x square.

This guy multiplied by T i comma k minus beta delta t T i comma k minus 30 was the value of T infinity, initially we will take value of beta to be equal to zero and value of alpha is 0.2 value of delta x is 0.4. So, these are the conditions for which we are going to use Microsoft excel. In order to solve this problem, we will take delta t equal to 0.1 and then we will take delta t equal to one, for value of delta t equal to 0.1, we will show that the overall scheme is going to be stable because delta t has to be less than 0.4, for the choice of delta t equal to one, we will show that this scheme is over all going to be unstable.

So, that is the first part we are going to do and in the second part what we will do is we will take the value of beta, we will change the value from zero and we will take a more realistic value and that value is going to be beta equal to 0.002, as we have written down over here.

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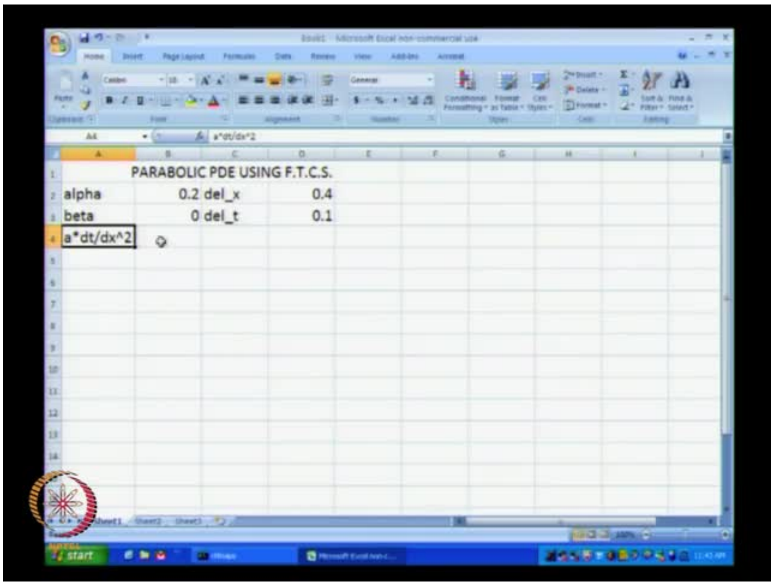

So, these are the three parts of the problem that will solve in three parts using Microsoft excel. Now, we are going to solve parabolic PDE, using forward in time central in space method. We will write our alpha value as 0.2 and we will write our beta value, initially it was zero. I will write our delta x values; delta x value we took as 0.4 and I will write our delta t value, sorry delta x value and delta t value, we will take initially as 0.1. What we need is we need to compute the value alpha delta t by delta x squared. So, we will compute that value also; so a into d t by d x squared, that value we will compute that because that is the coefficient that will need multiple times. For example, if you look at the board what we had solved.

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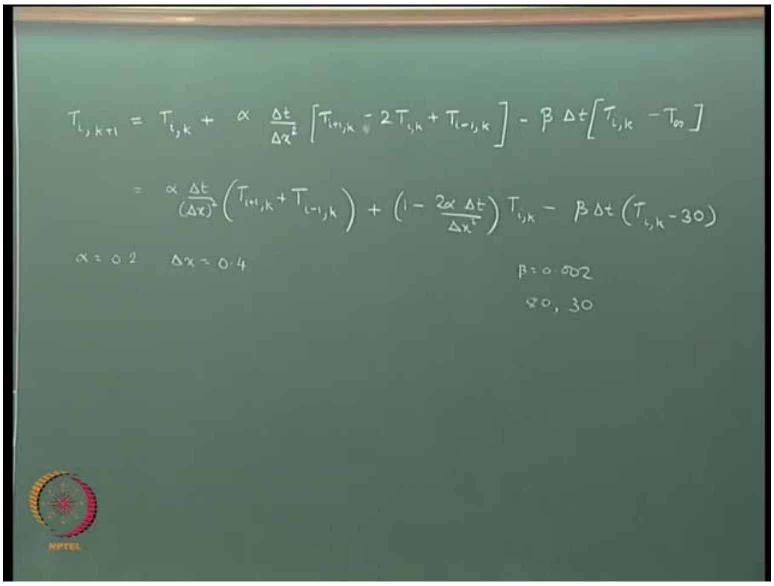

Now, if you look at the equation that we have then at several places, we require the coefficient. We require the coefficient alpha delta t by delta x squared over here as well as we require the coefficient alpha delta t by delta x squared over there. As a result, we will pre compute this particular coefficient alpha delta t by delta x squared, so that we can use this forward. Now, what we are going to do is we will start off with a temperature of 30 degrees along the length of the reactor that is going to be our initial condition and we will use this particular equation in order to update those values at every time.

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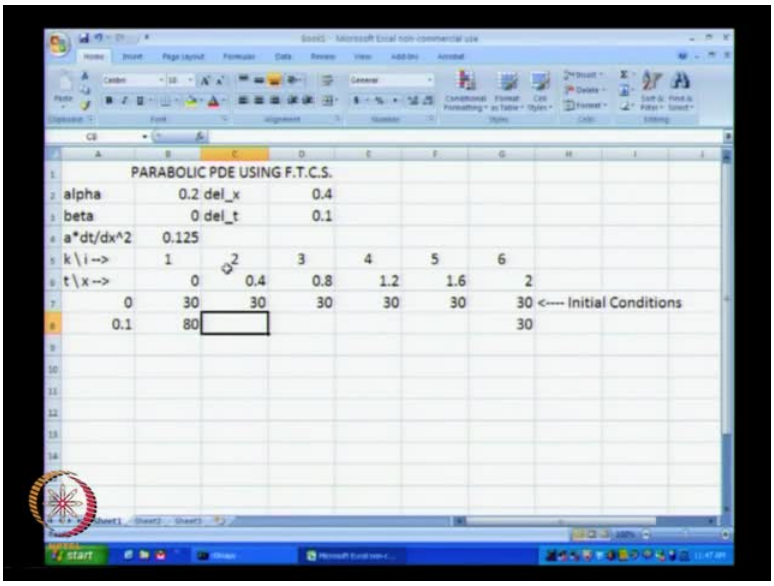

So, that is what we are going to do and let us go back to excel and we will compute our alpha delta t by delta x square and that is going to be equal to; so let us now compute our alpha delta t by delta x squared and that is going to be equal to this multiplied by delta t divided by delta x square. So, that is what we have as this particular value over here. If we were to use delta t equal to one that becomes 1.25 for delta t equal to 0.1 at 0.125 and that is the value of our a. So, now what we need is on the columns we will have the various temperature values along the length of the rod. So, I will have the locations, i specified along the columns and k will be specified along the various rows.

So, i will go along the columns, so i is 1,2,3,4,5 and 6, that is going to be our i's, I will just centre it or make that centered and we have initially at time t equal to zero, at time t equal to zero all the temperatures are at 30 degrees. So, I will write all of them as 30. So, these are our initial conditions. Starting with initial conditions, now we go forward as we move forward we will write these things down. I will move this one row below and I will actually write down the actual time and our actual x, I will write this.

This is going to be equal to zero. This is going to be equal to the previous value plus delta x and I will put the dollar signs over there because the delta x does not change. So, this is the length of the reactor or sorry the length of the rod going from zero to two centimeters. The time is going to be equal to previous value plus delta t and I will again press F 2 and put dollar sign, so that when we move, when we just drag it below, we do not, we would not have this value changing. So, what happens at time 0.1 is our initial condition changes, the boundary condition changes. At one end of the rod, the temperature is suddenly made a t and at all the other ends we have at sorry at the other end we have the temperature kept at 30 and we want to find out how the temperature changes for all the internal points ok.

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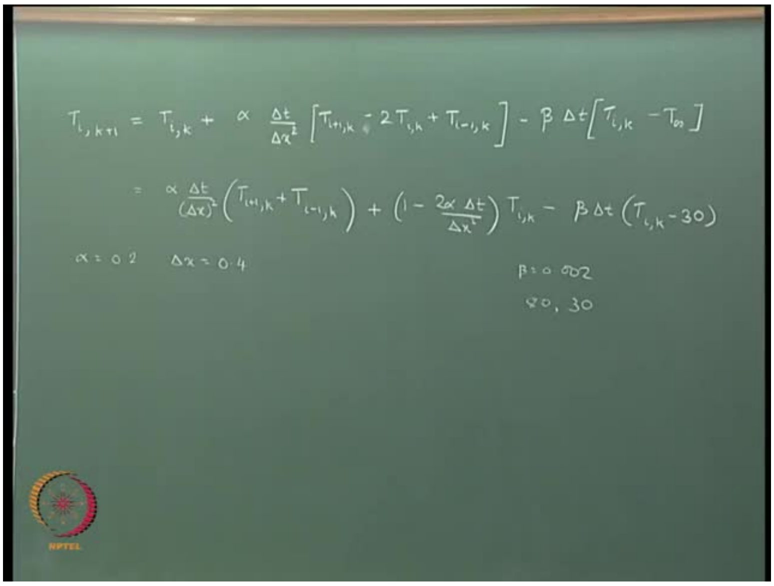

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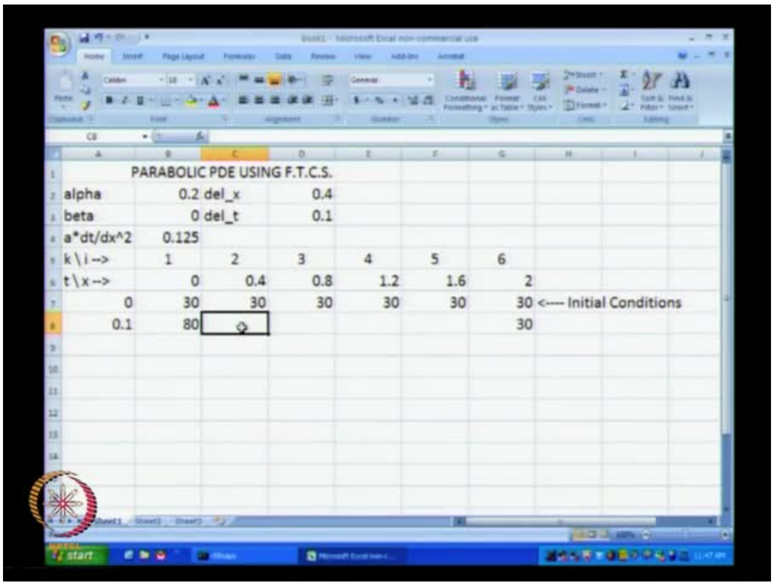

So, this is the temperature at this is going to be T i comma k is going to be equal to T 2 comma 2. Now, T 2 comma 2, if we look at the expression it is going to depend on the values of at the previous time, it is going to depend on this value, it is going to depend on this value and it is going to depend on this particular value.

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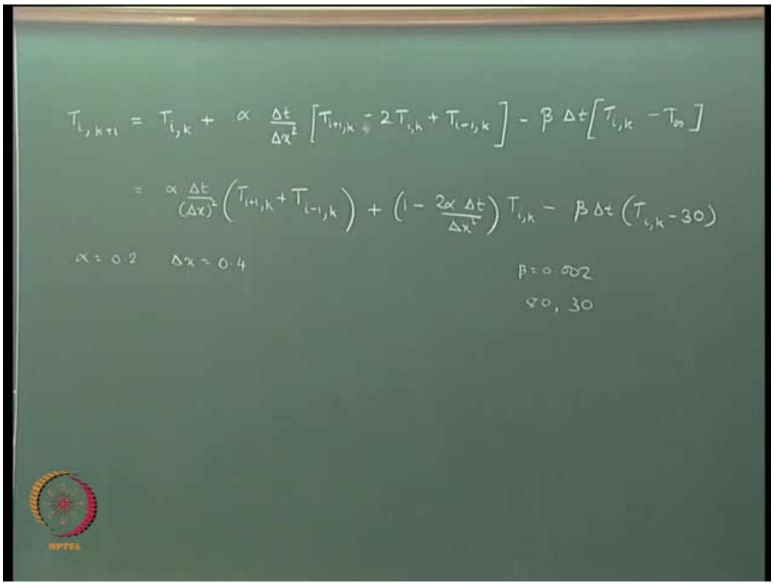

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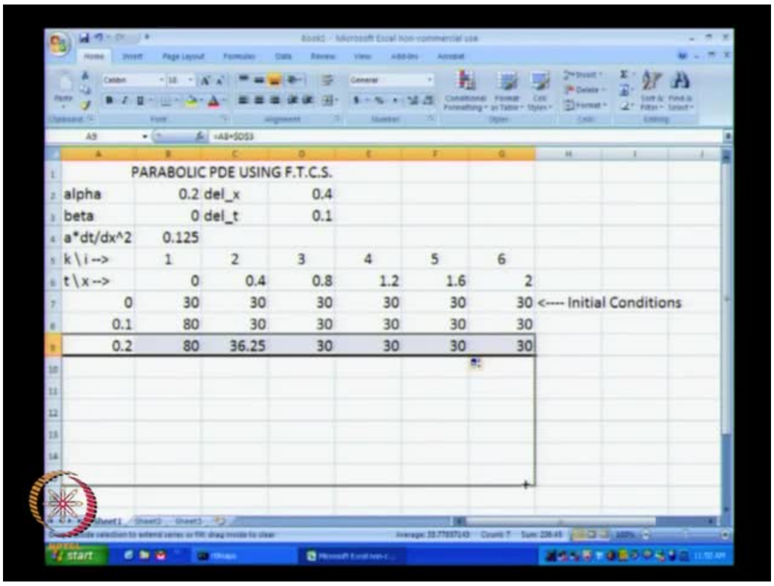

	PARABOLIC PDE USING F.T.C.S.						
alpha	0.2	del_x	0.4				
beta	0	del_t	0.1				
a*dt/dx^2	0.125						
k \ i -->	1	2	3	4	5	6	
t \ x -->	0	0.4	0.8	1.2	1.6	2	
0	30	30	30	30	30	30	<---- Initial Conditions
0.1	80	30	30	30	30	30	
0.2	80	36.25	30	30	30	30	

So, I will write that down as now what we had was alpha delta t by delta x squared. This multiplied by T i plus one comma k plus T i minus one comma k. So, it is alpha delta, so this guy is alpha delta t by delta x squared multiplied by T i plus one comma k, and this is T i minus one comma k. This is added to one minus two multiplied by alpha delta t by delta x squared. This guy multiplied by T i comma k so our T i plus one comma k T i plus one comma k was going to be equal to alpha delta t by delta x squared multiplied by this guy plus this guy plus one minus two alpha delta t by delta x square multiplied by this guy.

Now, we had that beta term also we will have that term coming in over there is well. So, we will just sorry what we are going to do is we are going to put dollar signs for our alpha delta t by delta x squared. then we can just drag it and then we will press F 2, we will see this guy as alpha delta t by delta x squared multiplied by T i plus one comma k plus T i minus one comma k, plus one minus two times alpha delta t by delta x square multiplied by T i comma k.

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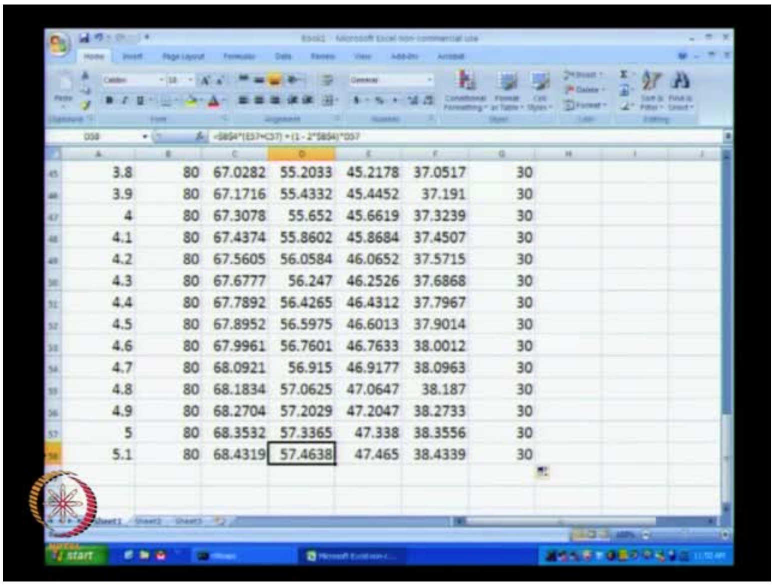

That is what we will get for the entire row. So, let us take this entire row and copy it say up to time five or something or time one or something. This is in not correct. What I will need is one more row and then I can move it down equal to the above value and this one is going to be equal to the above value and this one, I will just drag it downwards and that is going to be my temperature that we have and that we get at the time 0.2. And we just drag it at several locations and we go up to say time t equal to say five or something like that and I will just delete this.

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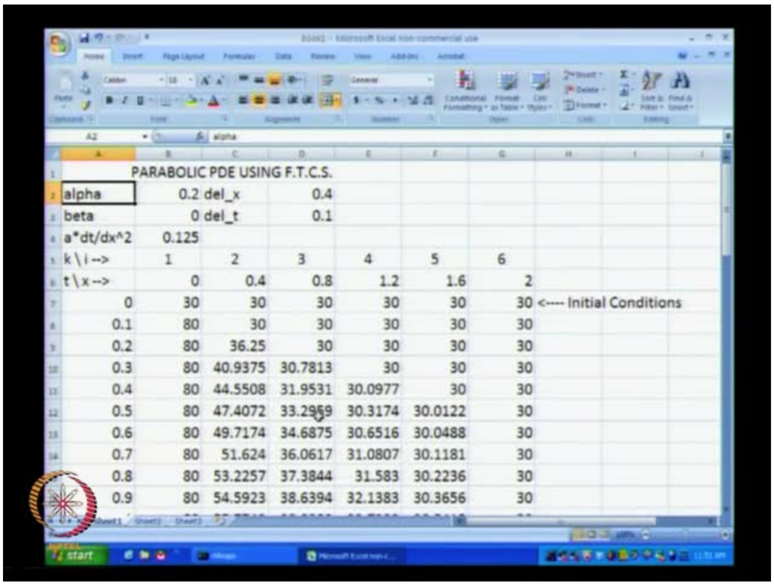

	PARABOLIC PDE USING F.T.C.S.						
alpha	0.2	del_x	0.4				
beta	0	del_t	0.1				
a*dt/dx^2	0.125						
k\i-->	1	2	3	4	5	6	
t\x-->	0	0.4	0.8	1.2	1.6	2	
0	30	30	30	30	30	30	<---- Initial Conditions
0.1	80	30	30	30	30	30	
0.2	80	36.25	30	30	30	30	
0.3	80	40.9375	30.7813	30	30	30	
0.4	80	44.5508	31.9531	30.0977	30	30	
0.5	80	47.4072	33.2959	30.3174	30.0122	30	
0.6	80	49.7174	34.6875	30.6516	30.0488	30	
0.7	80	51.624	36.0617	31.0807	30.1181	30	
0.8	80	53.2257	37.3844	31.583	30.2236	30	
0.9	80	54.5923	38.6394	32.1383	30.3656	30	

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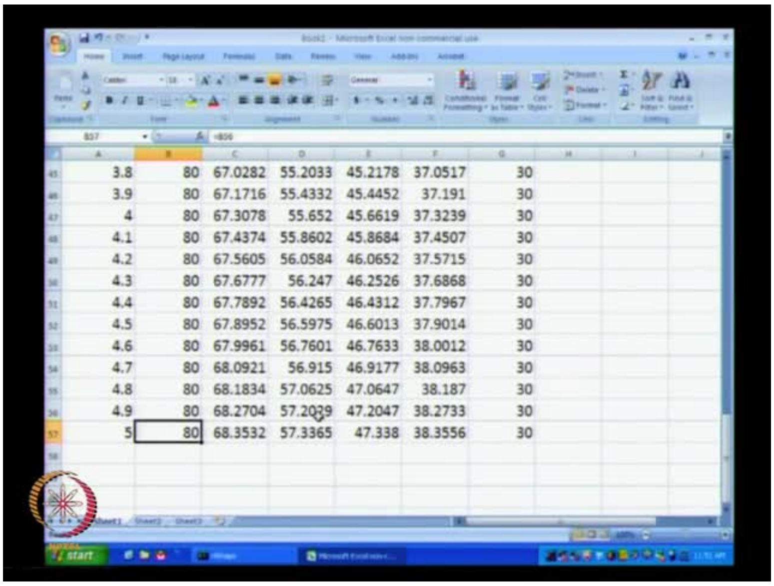

3.8	80	67.0282	55.2033	45.2178	37.0517	30
3.9	80	67.1716	55.4332	45.4452	37.191	30
4	80	67.3078	55.652	45.6619	37.3239	30
4.1	80	67.4374	55.8602	45.8684	37.4507	30
4.2	80	67.5605	56.0584	46.0652	37.5715	30
4.3	80	67.6777	56.247	46.2526	37.6868	30
4.4	80	67.7892	56.4265	46.4312	37.7967	30
4.5	80	67.8952	56.5975	46.6013	37.9014	30
4.6	80	67.9961	56.7601	46.7633	38.0012	30
4.7	80	68.0921	56.915	46.9177	38.0963	30
4.8	80	68.1834	57.0625	47.0647	38.187	30
4.9	80	68.2704	57.2039	47.2047	38.2733	30
5	80	68.3532	57.3365	47.338	38.3556	30

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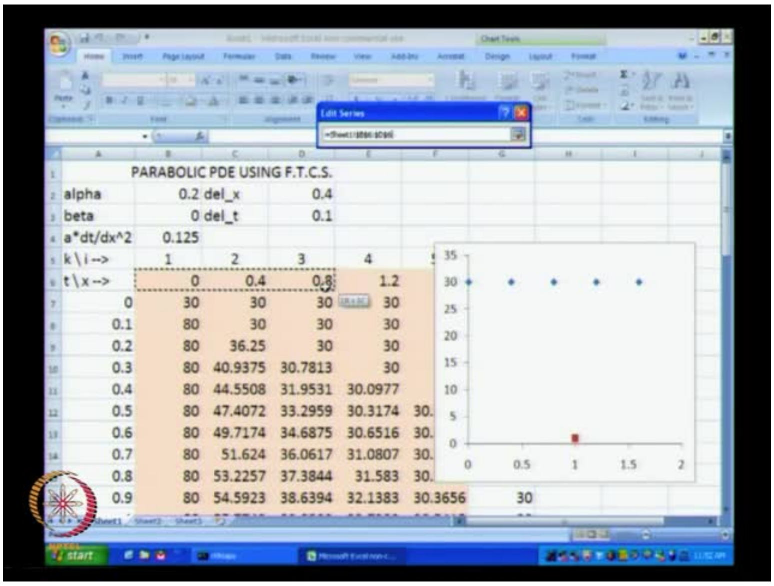

So, now what we have is we have the temperature at various locations, in the rod, as the time progresses. So, all these values that we have over here are the values of temperatures at various times, varying with various time and various spatial locations. So, these are the temperatures varying with time and space. So, what we will do is we will try to plot the overall temperature profile at various times along the length of the rod.

What we will do is we will select these guys as our temperature values. So, insert we will do a scatter plot, and will just delete this, we will delete this as series one. This is going to be our plot for our temperature which is all 30, changing with the location and I will just go here and increase the font size, so that the things are fairly visible so, this is the temperature at the initial point.

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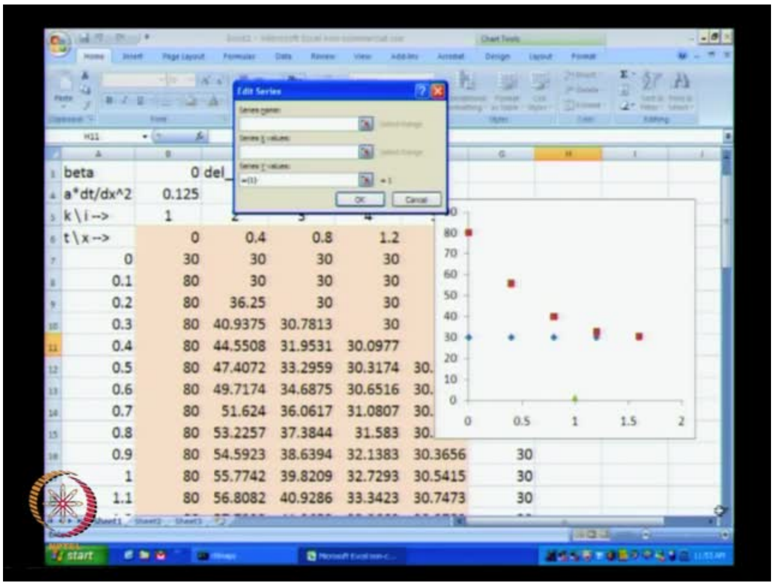

Now, what we will do is we will add some more data; select data we will do, we will add series. Now, what we need is the x values. These are going to be the x values. we will need the y values and the y values we will have them at time t equal to one second. So, this is going to be how the temperature looks like after one minute sorry after one second not one minute. Then we will have the temperature value along the length of the rod at the end of two minutes.

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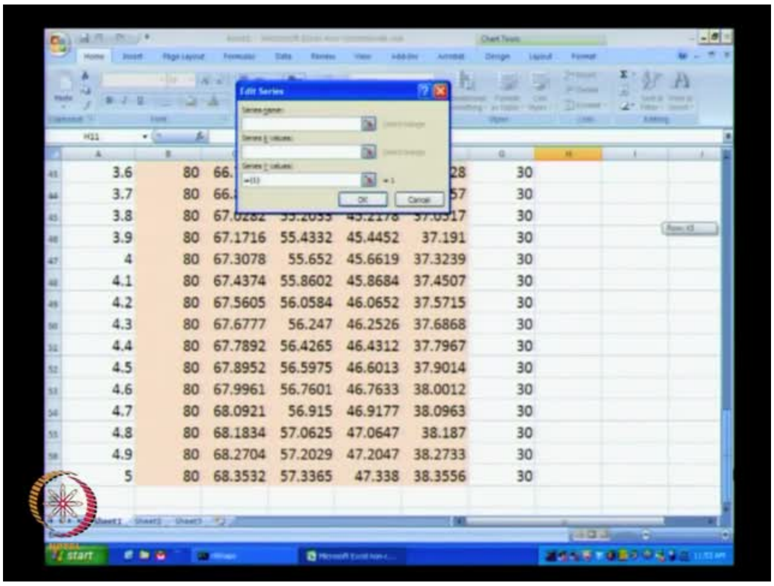

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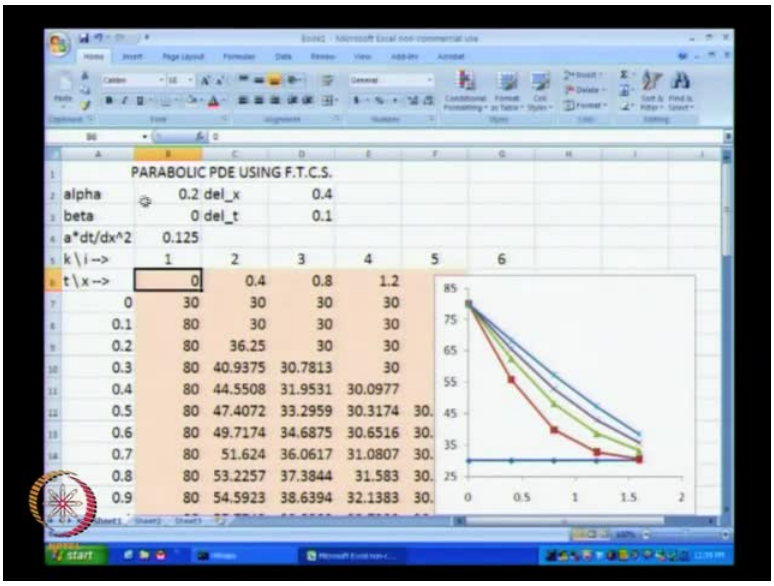

So, the y values should be these guys and the x values are going to be this. We will add one more series that would be at the end of we will just add one more at the end of three minutes sorry at the end of three seconds that is going to be this particular row and the x values, corresponding x values are at this row. We will add one more series at five. So, let us go up and look at the plot that we have obtained, go there, right click format axis and we will start the axis at say 25 and we will end the axis at say 85. We know for sure that the temperatures are not going to beyond 25 and 85.

So, that is what we will do. At format data series, we will add lines. (No audio between: 24:41-23:54). We will just add lines, so that we can see, fourth is going to be the fourth line and then finally, the fifth line. So, this is the temperatures along the length of the rod. So, this is the temperatures along the length of the rod at the initial condition. These are the temperatures at the along the length of the rod at after one minute. These are the conditions along the length of the rod and I will add a line over here also. So, this is how the initial condition is and this is how the final temperature is going to look like and this is how the temperature is changing along at various times along the location in this particular rod.

So, that is how the solution evolves. This is how the solution is evolving in time and this is how the solution looks like in space at various different times. So, this is the solution that we get when we have started over system at t equal to zero with using our delta t value of equal to one.

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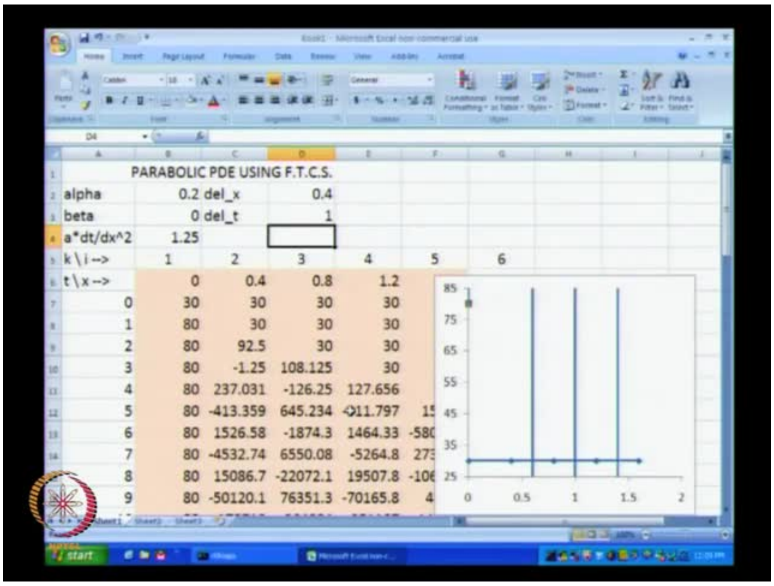

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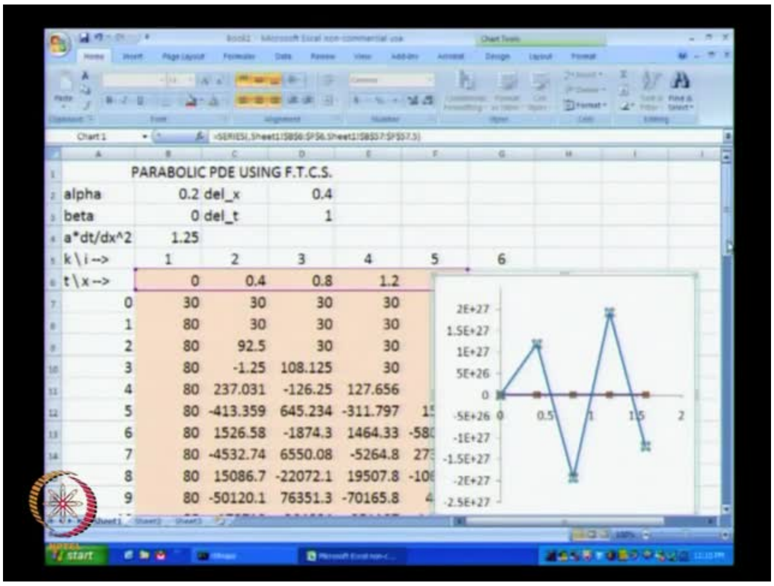

What happens let us see when we changed the delta t value equal to, from 0.1 we change the delta t value to one, and this is what is going to happen. We will just look at the various times at 0, 1,2,3,4 and 5. At zero, this is, just go and right click, format axis and I will have the minimum and maximum as automatic and we will change the data.

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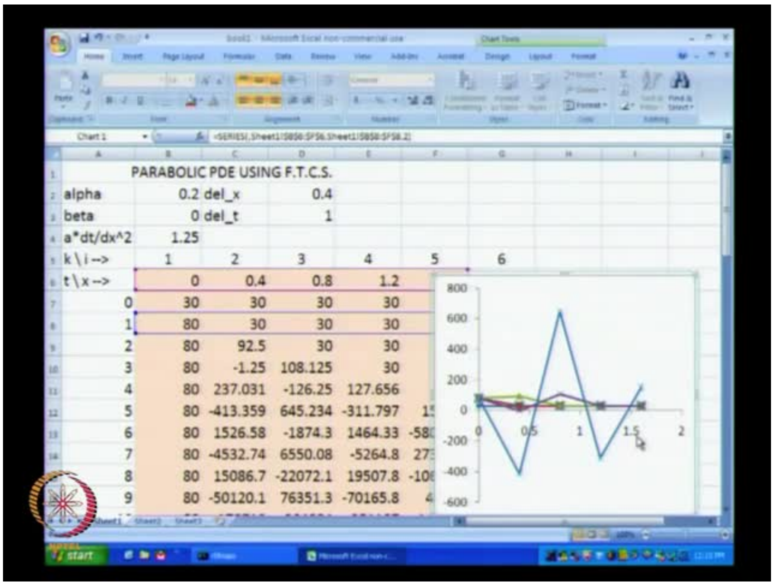

So, this is the data at five, this is going to be, I will just change the data and this is going to be the data at the end of three minutes. This is going to be the data at the end of two minutes, and the data at the end of one minute and this is the initial data. So, this is what we get, so at initial conditions, we had this temperature and you can barely see it the temperature was at 30 degrees. At the end of one minute, again the temperature is still well we have 80 degrees, 30, 30, 30 and so on. At the end of two minutes, we have 80, 92 degrees becomes the next temperature.

Now, the temperature cannot rise beyond 80. These 92 degrees that we see is definitely incorrect. At the end of three minutes the temperature goes negative, so at one end of the rod, the temperature is kept at a t. At the other end of the rod, the temperature is kept at 30. There is no way how the temperature should actually go below 30 degrees or should go above 80 degrees.

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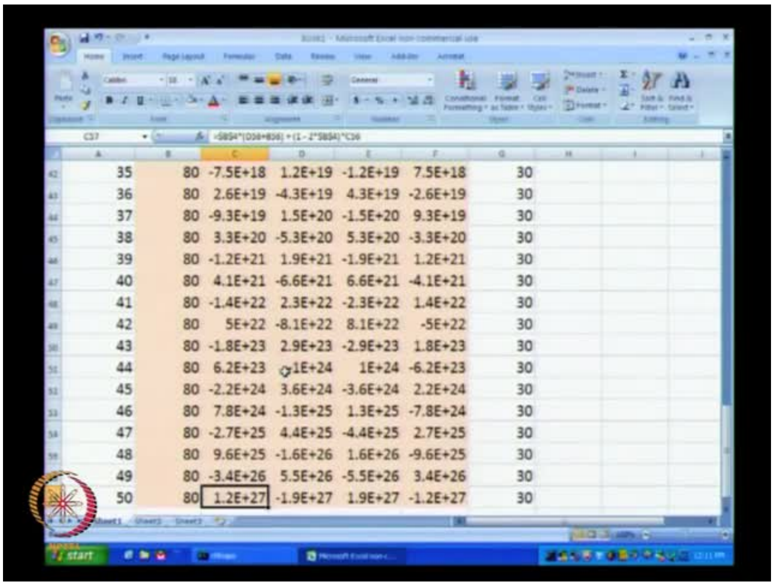

But that is what our module gives. At the end of five minutes, we have the temperature predictor as minus 400 and plus 600. If we look at what temperatures being predicted at 50 minutes, sorry, not fifty minutes but fifty seconds, we have temperature predictor as 10 to the power 27, minus 10 to the power 27 so on and so forth.

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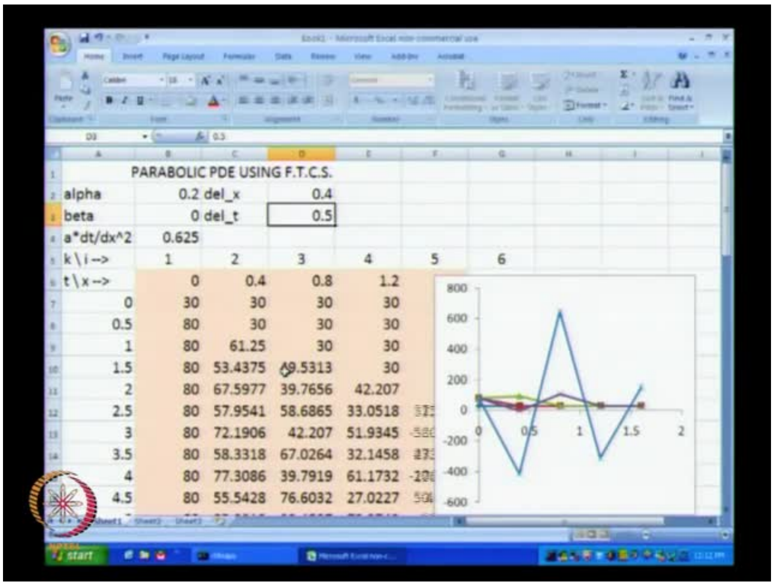

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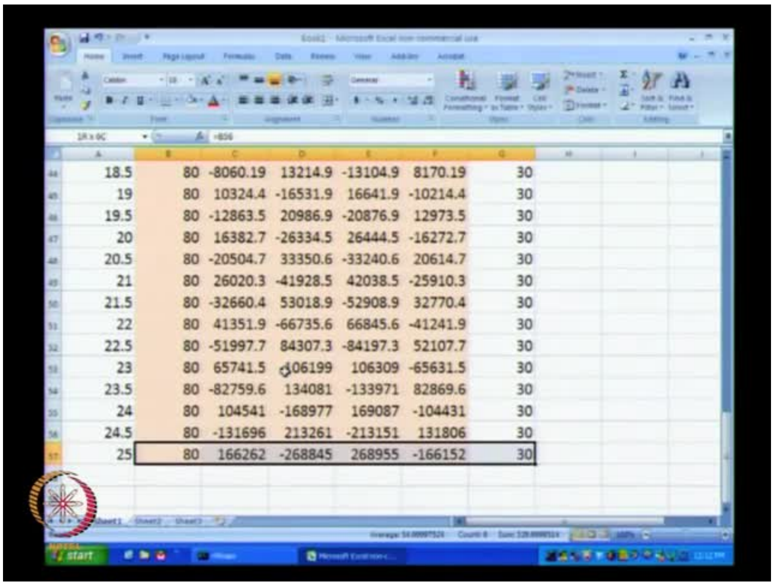

So, what we have seen is that when we go to delta t equal to zero from 0.1 to one, we get from stable solution, we will move on to the unstable solution. What happens when we take this delta t equal to say 0.5? Again we will get some kind of an oscillations and finally, this should, the temperature is going to be unstable that is what these temperature show you.

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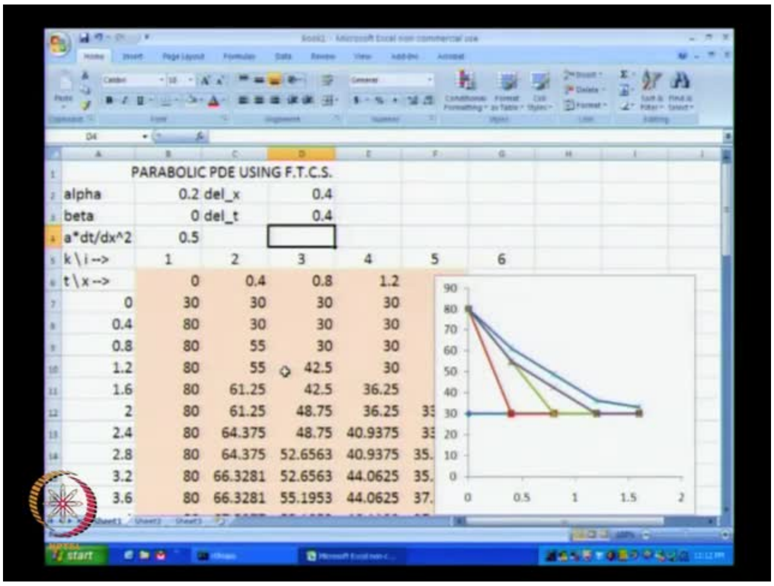

So, these temperatures are clearly we are going on to unstable region and what happens when the delta t is kept at four; exactly equal to four. We will get the temperature to be stable, the temperatures are not unstable but, the temperatures are indeed stable when delta t is 0.4. What happens when we go at 0.42 is we will get some kind of oscillations if you see over here. If we go to long enough time, you will see that the temperatures indeed are tending to diverge and not converge. We started with temperatures of 56, initially and then they are going to 70 and they are hovering around 69 and 70, so on and so forth.

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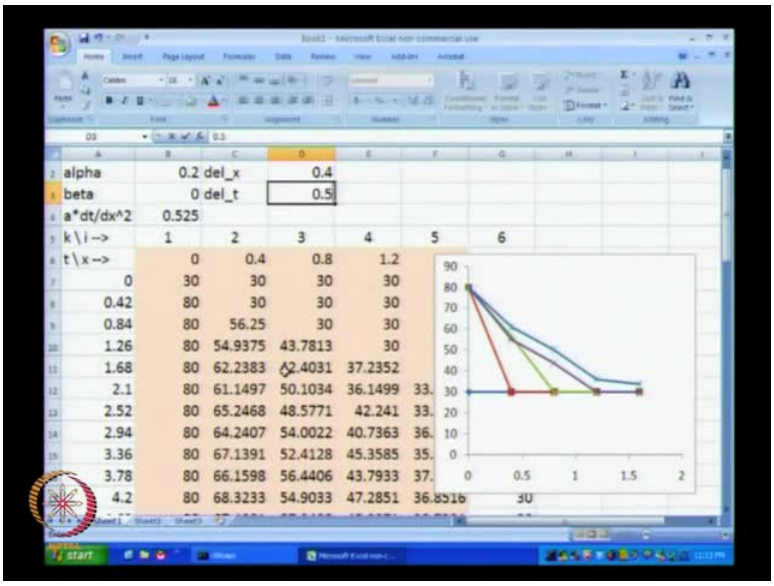

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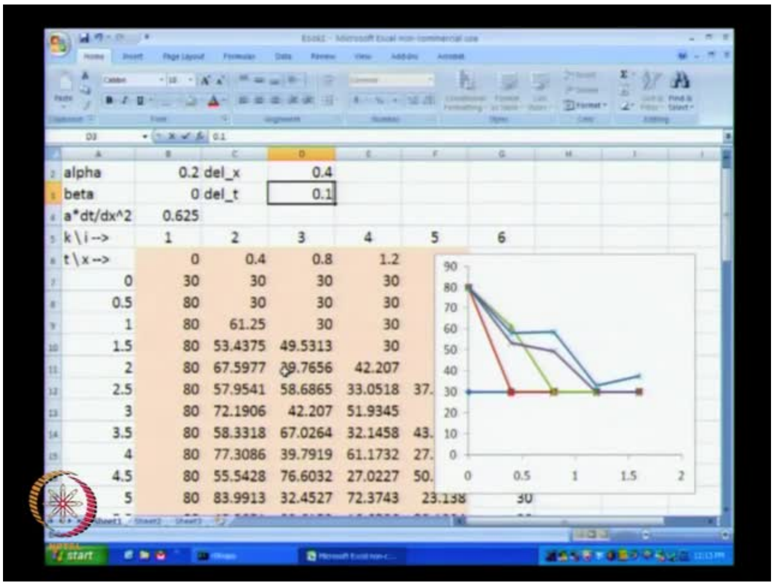

So, just to recap, we take a delta t greater than 0.4 and we will get our temperatures to be diverging. If we take the delta t less than 0.4, we will see that the temperatures are indeed converging at the end of our simulation.

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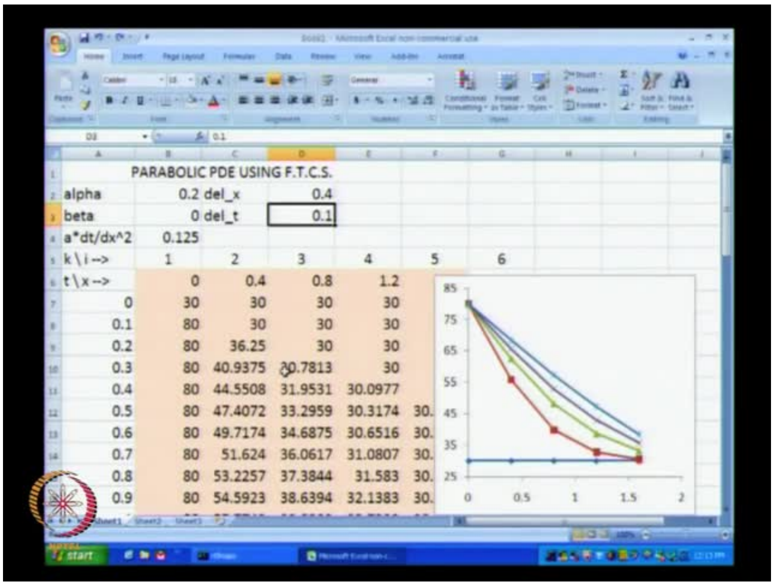

That is what we have seen using the forward in time central in space method, I will just press delta z several times, so that we get our final solutions. This was what our solution work at for delta x equal to 0.4and delta t equal to 0.1. So, I will just include the other temperature also in the final boundary where I had not included. So, we will just move this and same thing we will do with other temperatures as well. So, this is how our solution looks like when we have beta equal to zero, we take our delta t small enough so that we get convergence.

Now, when we change from our beta, from beta equal to zero to beta equal to 0.002, we need to go and change our equations that we have put for the expressions sorry that we have put for these conditions to include the effect of beta as well. So, we will go here and we will press F2. Now, this is without the beta term.

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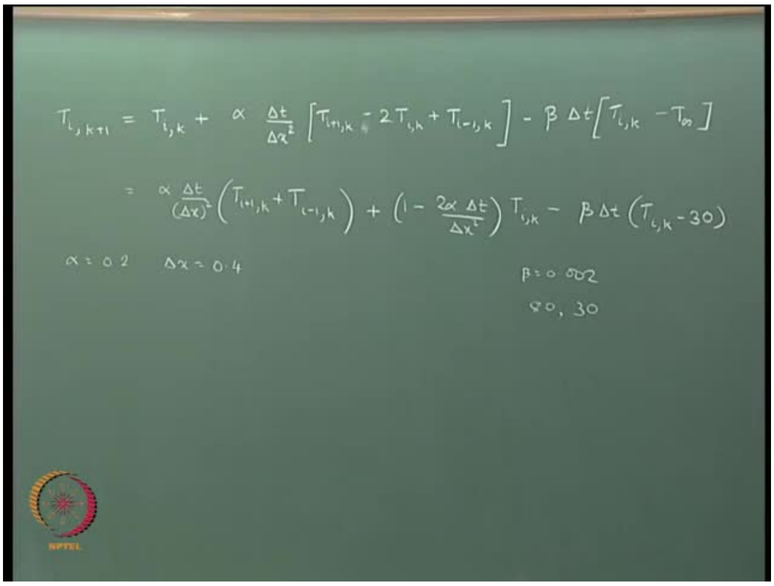

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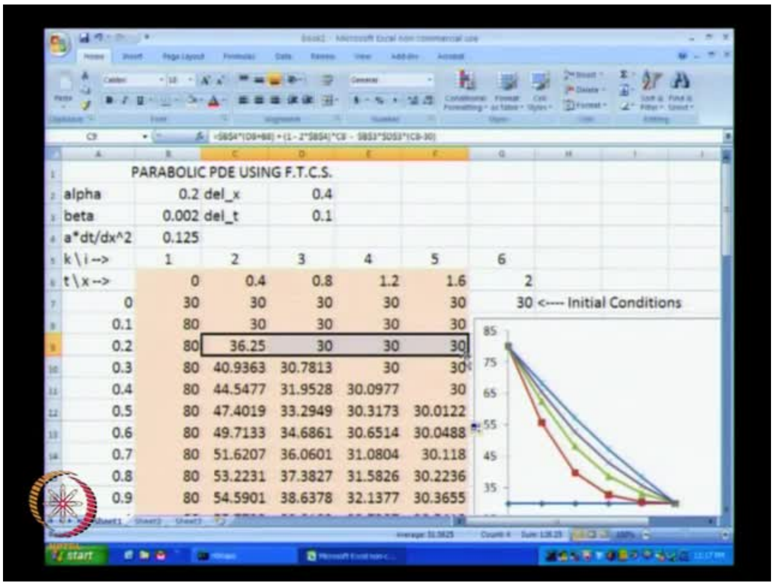

Now, if you look at the board, the beta term that we have is now we need to include beta multiplied by delta t multiplied by t minus 30. That is the term that we are now going to include, so minus, if you we had just seen. Now, minus beta multiplied by delta t, which was over here multiplied by a temperature i comma k, which is this guy, k remember over here is equal to one, our i is equal to two, so i comma k is going to be this guy minus 30 was the temperature of the ambient.

So, we will just put dollar signs over here dollar b, dollar three, because the beta value the self, the beta value is not going to be change, the self or delta t is also not going to change. It is going to remain over here. So, we will put dollar signs over here as well. We will just move this and copy it over here, and we will just go ahead and check one of this value. We will just drag them below and we will check one of the values. We will press F2 and check these values. This guy is going to be alpha delta t by delta x square multiplied by T i plus one plus T i minus one, plus one minus two times alpha delta t by delta x square multiplied by T i comma k minus beta.

That is over here multiplied by delta t that is over here multiplied by t the temperature minus 30 that is the temperature at the ith location minus 30. That is the expression that we had to get, so we will select all this and double click, so that all the values below are going to change. What we see over here for that small enough value of beta that beta does not affect the overall temperature profiles; almost there is almost no effect on of beta on the overall temperature profiles that we get in this rod. There is only a very slight change.

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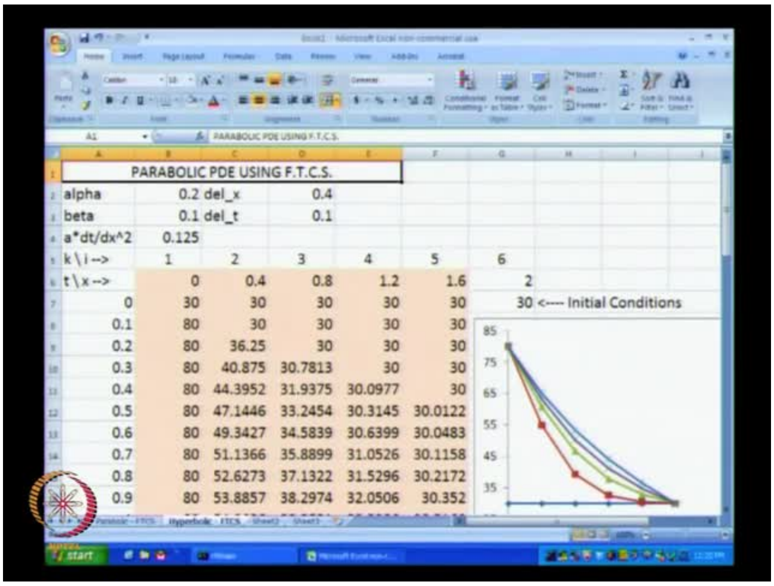

Now, let us change from beta equal to 0.002 to 0.01. We see that temperatures have change very slightly and then when we change that beta to 0.1 we find that the temperatures have changed quite a bit again. So, when beta was equal to zero this were what the temperature profiles were. When beta we had changed to 0.1 this is what the temperature profiles are. So, what is happening when we change the beta really is we are seeing the effect of heat loss taking place from the outer ends of the rod to the surroundings. This is what the effect we are going to get. So, what we have done now using excel is basically talk about the parabolic PDE solving using forward in time central in space method. The other methods for solving parabolic PDE were central in time, sorry were backward in time central in space, and that is going to be a fully implicit method of solving. So, we have forward in times central space, which is going to be first order accurate in time.

However, it is going to be an explicit method for solving these equations. The next method is going to be basically backward in times central in space, which is a fully implicit method and the third method that we had talked about was the Crank-Nicolson method, which is an implicit method, but it is second order accurate in time. So, those were the methods that we talked about for parabolic PDE.

I will just rename this particular sheet as parabolic and FTCS. What we will next do is we will do this exercise for hyperbolic PDE and I will just move or copy this particular sheet, the sheet before, create a copy and we will retain most of it; however, we will change this to hyperbolic and what we expect in hyperbolic equation is that we will get the system to not converge in this particular example. We will go and look at that example on the board and then we will try to solve this.

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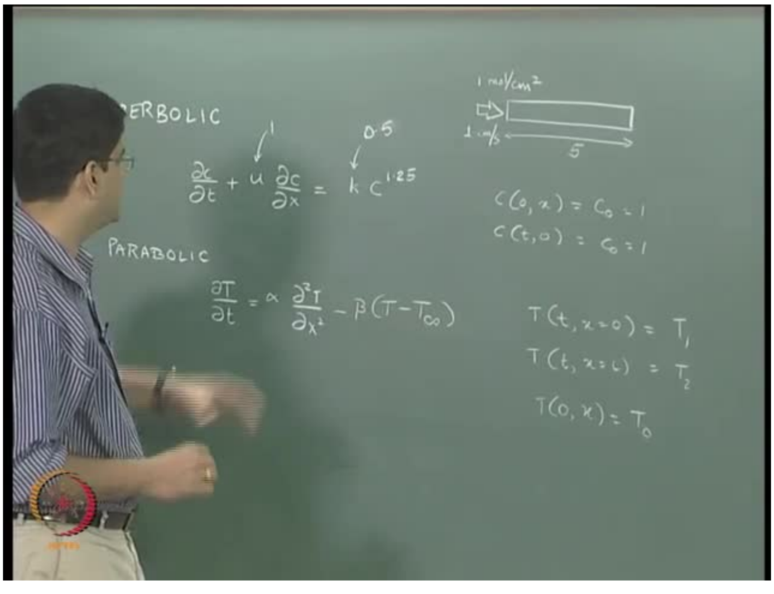

So, the hyperbolic equation that we had was d c by d t equal to u d c by d x, sorry plus u d c by d x equal to k c to the power 1.25. From the previous time, basically, we had taken our k value as equal to 0.1 and our u value was.. sorry our k value was equal to one. I know, I think yes, the k value was equal to 0.5 and the u value was equal to one. we were trying to look at the overall reactor of length five centimeters.

So, the overall reactor was of the length five centimeters, the inlet concentration was one moles per centimeters square and inlet velocity was one centimeter per second. Our k value was 0.5 moles per centimeter cube to the power minus 0.5; sorry minus 0.25 divided per second and that was the k value. So, for these conditions we will go now and try to solve this equation. Before doing that we will just express this as we did before with parabolic FTCS.

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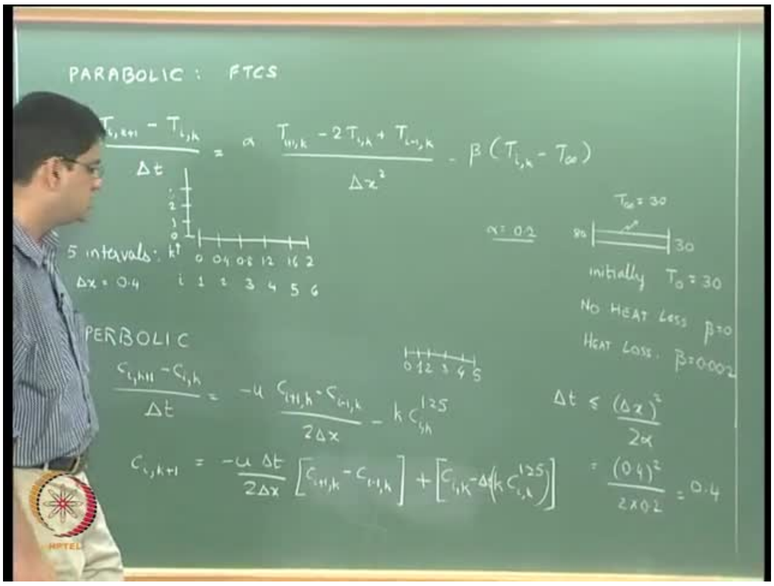

So, we have what we have over here is the derivation for the parabolic FTCS. We will do the same thing for the hyperbolic equation. for hyperbolic, we get c i plus one sorry c i comma k plus one minus c i comma k divided by delta t, is going to be equal to minus u multiplied by c i plus one comma k, minus c i minus one comma k, divided by two delta x, minus k multiplied by c i comma k, to the power 1.25. If we go back to this equation, actually I had made small mistake over here, (Refer Slide Time: 39:37) there should be a negative sign that should appear, because as the reaction takes place, the amount of the concentration of that the reactant starts getting depleted from the system.

So, there should be a negative sign over there, which I had missed. Now, rearranging what we what we will get is c i comma k plus one. Now, we multiply by delta t and we take c i comma k on to the other side, so we will get c i comma k plus one should be equal to minus u delta t by two delta x multiplied by c i plus one comma k, plus one minus u delta t divided by two delta x c i. sorry, that is not right (Refer Slide Time: 40:37) minus u delta t divided by two delta x multiplied by c i plus one comma k, minus c i minus one comma k, plus c i comma k, minus k times c i comma k to the power 1.25. So, this is what we would be getting and there should be a delta t term over here, so minus delta t multiplied by this guy.

So, this is the overall expression that we will get by doing the substitution. The initial condition is that the temperature is sorry the concentration is going to be one throughout the reactor. The inlet condition is that the concentration is going to equal to one throughout the reactor and this is the equation that we are going to indeed employ in order to solve this overall problem. So, let us again go back to excel and modify the PDE, the parabolic PDE excel sheet that we had previously used for this hyperbolic equation, where again the values of u, was equal to one. Our delta t, as before, we will take our delta t equal to 0.1. Our delta x, in this particular case is going to be equal to one, because we are going to divide length five into five interval's. So, from zero to five, we will divide into five intervals that is going to be our delta x.

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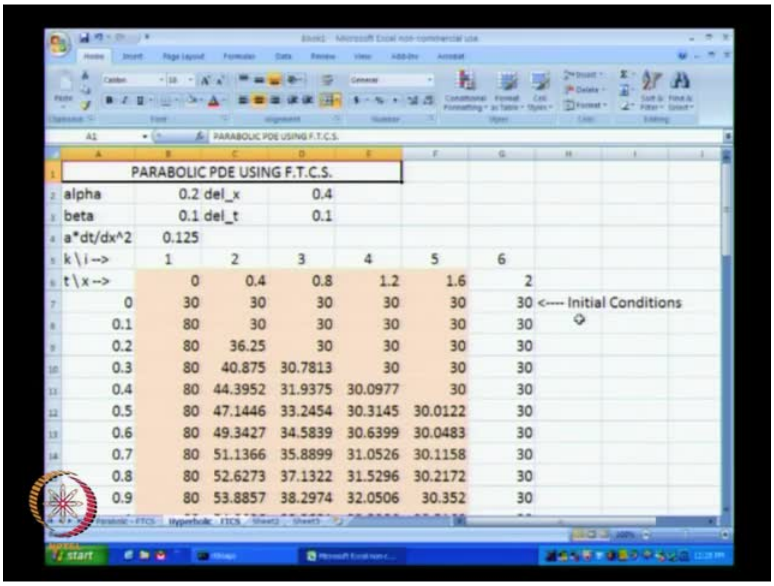

PARABOLIC PDE USING F.T.C.S.							
alpha	0.2	del_x	0.4				
beta	0.1	del_t	0.1				
a*dt/dx^2	0.125						
k\i-->	1	2	3	4	5	6	
t\x-->	0	0.4	0.8	1.2	1.6	2	
0	30	30	30	30	30	30	<---- Initial Conditions
0.1	80	30	30	30	30	30	
0.2	80	36.25	30	30	30	30	
0.3	80	40.875	30.7813	30	30	30	
0.4	80	44.3952	31.9375	30.0977	30	30	
0.5	80	47.1446	33.2454	30.3145	30.0122	30	
0.6	80	49.3427	34.5839	30.6399	30.0483	30	
0.7	80	51.1366	35.8899	31.0526	30.1158	30	
0.8	80	52.6273	37.1322	31.5296	30.2172	30	
0.9	80	53.8857	38.2974	32.0506	30.352	30	

So, let us now solve this overall hyperbolic equation using Microsoft excel. We will just modify the parabolic PDE we using FCTS appropriately.

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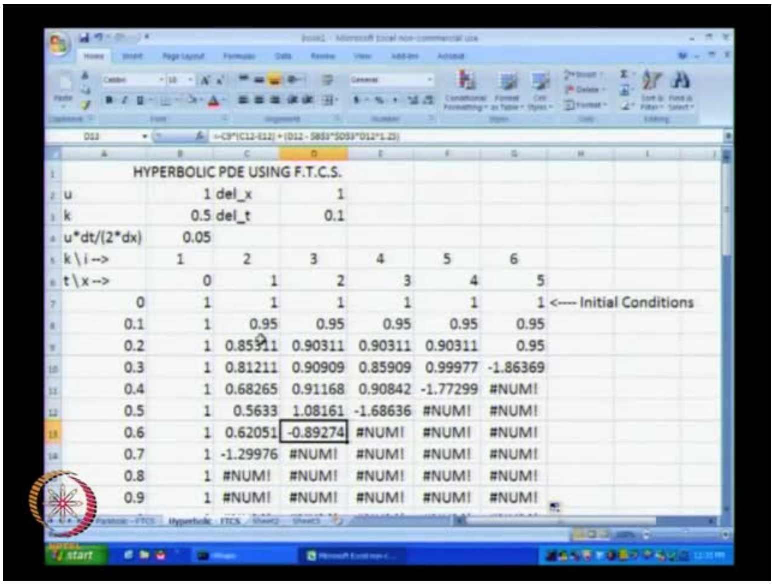

So, let us look at excel now. Hyperbolic PDE using FTCS, now what we have instead of alpha, we have the velocity u and the constant k. the k is 0.5, over here u was equal to one, del x we have taken as equal to one, and delta t we will take 0.1. We do not need alpha delta t by delta x square, as we had previously. We will, instead of alpha delta t by delta x square, what we need is u multiplied by delta t, divided by two delta x k. This is what we actually need, so that is what we are going to compute.

So, this is going to be equal to u multiplied by delta t divided by two multiplied by delta x. That is the value that we are going to use over here, and this are the x locations and this is the actual length of the reactor that we have. These are going to be the times, various times, so I will just select this and what I do not want is any fill, anything to be filled over here. I will delete now. Initial conditions, throughout we had 1,1,1,1 and 1. Those were going to be our initial conditions and what we have over here is basically at the inlet, our values do not change.

So, these are going to be the inlet conditions, so we have the initial conditions over here. We have the inlet conditions in this particular row. Now, using the equation what we have is equal to minus u delta t by two delta x multiplied by we have this previous value plus the next value in the location. So, that is really what we are going to get over here and using that value plus we will have c i comma k minus k multiplied by c i comma k k multiplied by c delta t multiplied by c i comma k, is what we are going to get to the power 1.25.

So, what we have over here is we have minus u delta t by two delta x, multiplied by T i plus one comma k, plus T i minus one comma k, plus sorry, not T It is going to be c i plus one comma k and here we have c i comma k minus k, which is the constant. we should put dollar signs over here dollar b, dollar three, that remains that stands for this particular constant and k multiplied by delta t. Again, we put dollars over here multiplied by concentration at i comma k, to the power 1.25 and this is what we are going to going to get up to here. at this particular condition, we will have to really use some kind of backwards difference formula, we cannot really use the central difference formula, simply because there is no boundary conditions that that should be satisfied over there.

So, the backward difference formula at this particular location is just basically going to look like minus u delta t divided by delta x, so it is going to be two multiplied- it is going to be equal to minus two multiplied by this particular guy, multiplied by c i minus c i minus one, plus c i comma k minus k times delta t times c i comma k to the power 1.25. That is what we are going to get over here. Just made a small mistake, (Refer Slide Time: 47:54) this should not be a plus sign, this actually should be minus sign, because that is what derivative is going to be about and that is what I want to drag.

So, these are the values that we have obtained and let us just double click and just drag and drop. So, what happens over here is that the concentration values soon to become negative, so we have this as a negative concentration here. We get a negative concentration here, we get a negative concentration, as a result of this soon we will have the overall scheme failing. But, even before it fails what we know is happening over here is we know for sure that the concentrations are going into negative, which is not a physical phenomenon. So, what we see in this particular case is that the forward in times central in space method does not work for hyperbolic PDE.

So, this is where I am going to end today’s lecture. What we have done in today’s lecture is look at forward in time central in space formula using Microsoft excel and applied to parabolic and hyperbolic PDE. The thing we are said about the parabolic PDE's is we need to check the value alpha multiplied by delta t divided by delta x square.

Now, that particular value, if that lies between minus half and plus half, then our overall scheme is going to be stable and if that lies beyond minus half and plus half, our overall scheme is going to be unstable. When we implemented that what we found was that the delta t value has to be less than 0.4. So, we took several examples, in one case we took delta t value was 0.1, in another case we took delta t equal to one, and in the third case we took delta t equal to 0.5. What we saw was for delta t equal to 0.5 and delta t equal to one, the overall solution went to 10 to the power 27 or something like that the temperature predicted by our code was 10 to the power 27, which are clearly not physical physically possible. They are clearly not numerical possible from this particular actual equations.

So, what that means is that the numerical solution that we had used was an unstable method, the numerical method that we use was unstable method for delta t greater than 0.4. Then we used a hyperbolic PDE, we use the same forward in time central in space method and for delta t equal to 0.1, also we found that the forward in time central in space method does not converge.

So, what we are going to do in the next lecture and which is going to be the final lecture in our computational techniques course is use the upwind method for solving the hyperbolic PDE and we will see that the upwind method converges under certain conditions and that is where we will end our discussion on PDE. Basically, solving the parabolic and hyperbolic PDE is essentially where we end our lecture series on that and then we will recap what we have done through all the modules in this particular course.

Thank you and see you in the next lecture.