Quantitative Methods in Chemistry
Dr. Aasheesh Srivastava & Dr. Bharathwaj Sathyamoorthy
Department of Chemistry
Indian Institute of Science Education and Research - Bhopal

Module No # 06
Lecture No # 26
Simulating simple straight lines and kinetic curves using MATLAB

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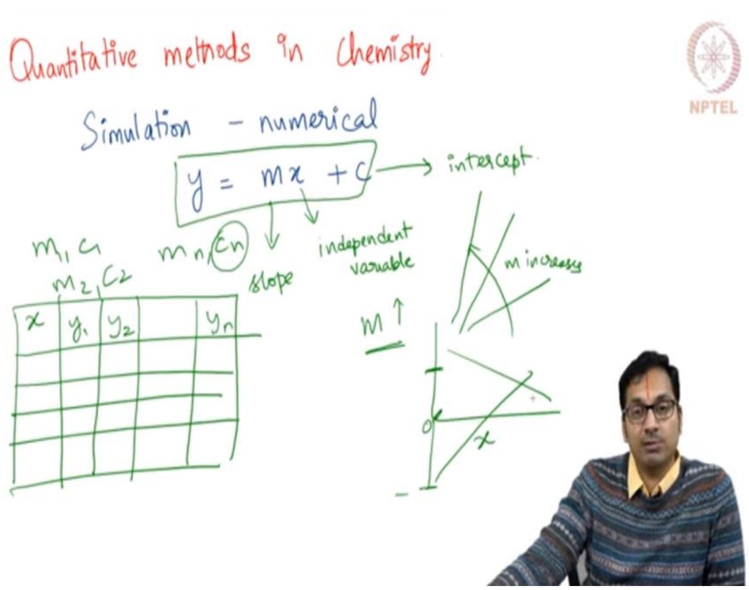

Welcome to the next lecture in quantitative methods in chemistry. In the previous week of lectures we were able to see how software could be used to save your data and also could be used to do basic data analysis in terms of linear fitting, nonlinear fitting and data analysis similar sort. In this week of lecture we will be trying to use more of a competition program like a MATLAB instead of what we use last week.

We ended up using a lot of spreadsheet last week. But here we will be using a software called MATLAB where we can try to do even larger scale of data analysis. And before doing that I felt it will be a good idea to introduce you to the syntax of a MATLAB and what is the big deal about using a software of that kind. In order to do that we will be doing simple simulations basically numerical simulation where we will be taking a certain model type and trying to generate numbers and take a look at how do they behave and how do they look.

The simplest numerical simulation that we have quite comfortable with is the straight line equation which is y = mx + c I am sure we have seen this a lot. Where the m stands for the slope, the x is the independent variable and c is the intercept. So now if I give you a bunch of values for x and a given value of m and c what is going to end up happening you can actually predict what is the value for y?

Now, let say that I will give you another set of slopes and intercept let say m2 c2. You can once again calculate y basically using the same equation and but with different values of the slope and the intercept. One can imagine that we can have different set of combinations of slope and intercept I need not need to understand how does the straight line look and behave. This math we have a good exercise to do so that when we understand as the m value changes let say it increases the slope of the curve increases right.

As you go from here to here m increases on the other hand if it could also be that the slope is negative in which case the slope is going to have a trend that looks like this on the other hand in this case if the slope is positive it going to have a different trend altogether. Similarly is the case with the intercept what we are able to understand is that if the intercept is 0 it will start at 0, 0 but if intercept is let say +c it starts here and if let say -c it starts over here.

And what you are able realize is that for different combination of m and c you can generate a lot of straight lines. Why I am saying this? This is I am saying this because this is something that everybody can relate with and we will start by understanding how the competition program something like MATLAB could help us to simulate something that is much more little more complicated.

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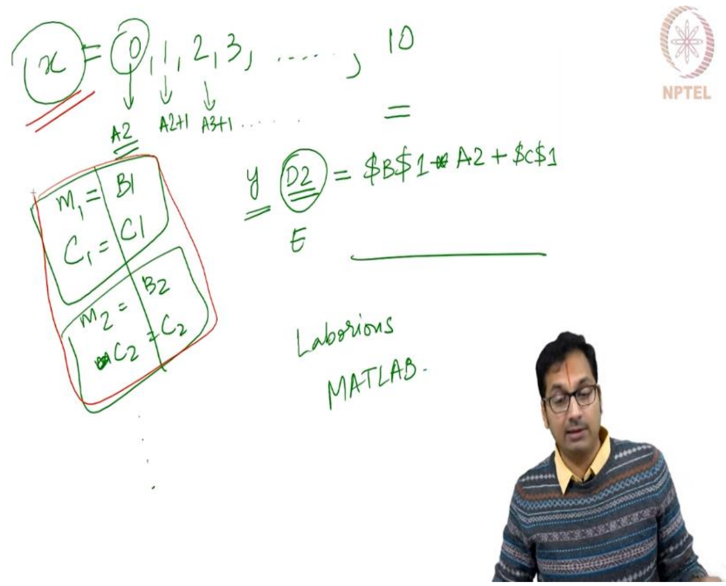

So we are going to take up the first example and before doing that we have to define a few set of syntax in MATLAB that we will end up using. Just the way we said x can be define as a variable let say you want to have 0, 1, 2, 3, and as 10 different number. In a the spreadsheet what we will end up doing this will be in the first row and you can always say let say row A2 you can always say A2+1 and this will be A3 +1 and so on.

So that these numbers can be autogenerated the moment you give the first value. Same would be the case if you are trying to use the spreadsheet where you will give m certain cell let say B2 and C ends something like C2 then we can try to determine all of the y value and say the column of D2 where we will try to end up saying let us say this also started from let us say these two are given in B1 and C1 where the value starts from A2.

So the D2 will be given something like dollar B1 sorry dollar B dollar 1 star A2 + dollar C dollar 1. And then what can happen you can generate all the laymen values for y by doing this. So similarly what is going to end up happening if you want to have another set of slope you could get that slope in B2 and C2 as C2 itself in the cells C2 and you can do something similar where you can do E and you can define this.

But remember what you are doing is that you are doing it for 2 sets or a given sets of a slope and intercept. So of course, this exercise can be repeated for a person to understand how a straight line looks and what is going to end up happening is to keep on doing it all this. Instead of doing this in a laborious way we can use computation software like a MATLAB to do the same. Of course this also involves similar parameter such that you will have to redefine the value x and then after you redefine a single or a bunch of values for m and then make it calculate.

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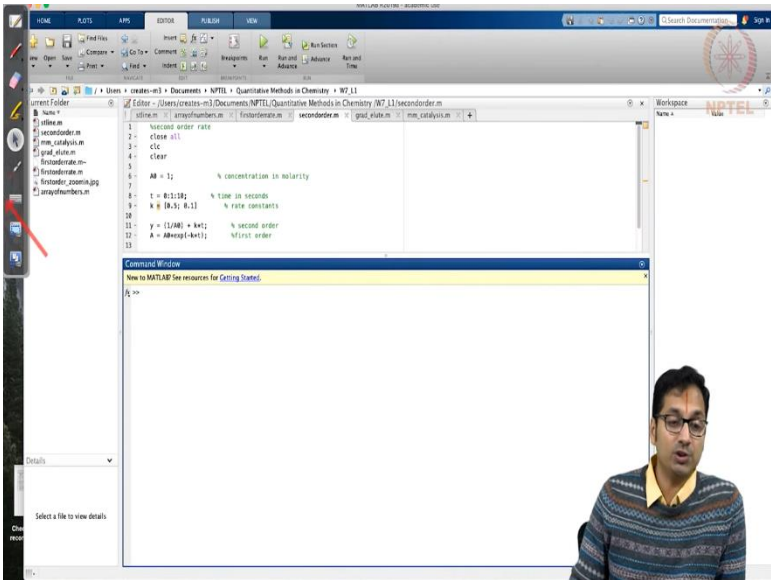

So why do not we quickly take a look and how this can be done using MATLAB and once again the purpose of doing this is to understand the syntax for MATLAB. So when you open the software MATLAB you have different portions that are exposed here. You are basically in a given folder which can be determining by typing the command pwd which stands for print working directory. Which is very similar to the Linux actually same as the Linux command.

And within that folder you will be able to see the different MATLAB files that you have written. In this case I have shown all the files up here so that it can see this is where the editor is basically when you are editing these files with the MATLAB you will be able to see them in a nice colored format. So that you can understand what is the command? What is the variable and what is the string and all the of that sort?

As we just saw what are files that here and how the editor is this is the terminal window where you type command. For instance you type the command pwd if you want to go to a certain directory you type c d and name of the directory. Here is also where you will be declaring variable. Let us take a simple variable like x ok let us actually not even call it x, you can call it anything. So let us call it fred, so you can call a variable fred and if you give an value 2 and hit enter then MATLAB says fred is the assigned value 2.

You can also say something like book = 4 then it assigns book as 4 and you can always add fred + book in this case you cannot say fred is reading a book here you would say fred + book is 6 because fred is assigned a value 2 and book is assigned the value 4. And here you will able to realize the simple arithmetic addition is performed between 2 and 4. You might always argue saying that ok why I am doing this? This can be done with the calculator you going to be saying that how this can be expand across a lot of numbers.

The commands clc stands for the fact that you are clearing the screen and then there is one important space that is here which is called a workspace and in the workspace you have all the different variables which is just define fred, we just defined book and you realize what is the value assigned for fred and what is the value assigned for book? Similarly all different variables are also assigned it is always a good practice to clear all the variables before we start working.

So if we hit clear you realize that in the workspace all the values are cleaned up. So once again let us say if you want to give x + 0 then x takes the value 0 and that appears here. And in the case we are trying to understand here we want to generate a set of number for x and in which case you can say x = 0, 1, 2, 3 of course with the space which indicates that these are different elements within an array in this case a matrix this is 1 / 10 matrix 1 / 11 matrix.

So if you do this x assigned gets assigns the variable of this sort. Of course we want to make our life easy so in which case there are library function in MATLAB which helps you to do that. So you can either say 1, 1 until 10 or rather 0, 1 until 10. So this is the short form notation for this where we try to save the initial value 0 and the final value is 10 and I would like to generate numbers with the increment of 1. You could do the same thing with the increment of 2 where you realize 1 is 0, 2, 4, 6, 8, 10 are generated.

The same thing can be done with other parameters like linspace where you try to say where is the starting point? Where is the ending point? And total number of numbers. And if you are able to realize as you keep typing the command MATLAB already suggest you how to use this. For instance if you using linspace x1, x2 that means when you say linspace 0, 10 it will generate numbers at a certain interval.

And how many numbers it has generated by default it has generated 100 numbers between 0 and 10 this is not what we want. We wanted to generate x as 1 integer units. So let us try to say x = linspace as you are typing this once again you have other recommendation that come you also have your way where you can define in what is the starting value of x1 what is the final value in x2 and the how many number of digit you would like to have which is n.

So in this case we want to have a 0 10, 11 you going to have 11 numbers between 0 and 10. And if you (()) (10:59) what you get is that x between 0 and 10 in 1 integer units. So what you have seen here is that you can generate the same 10 integer units by using different commands and there is always an easy way of finding all these if you go the internet and search for how to generate numbers or how to increment certain number you will easily able to find because the online forums are fantastic.

And there is one thing that we can do here is that we instead of displaying every value that comes if you use the semicolon what ends up happening is that the it is just does not display this certain values that are generated for this variable x. So now if you hit entire you realize that this numbers are not printed and of course the work space has created the number here just for the sake of understanding you can actually add between 0 and 20 and you would generate 21 numbers and then you will able to see here is that x is a 1 / 21 matrix ok.

So now that we have generated this next thing that we would like to do is to define a certain slope. As define a slope of 5 units m and we can define the intercept of let say -2. So now you have defined all of this now what you would like to do is to calculate y which is mx + c m star x + c. Of course if I do not give semicolon it is going to print the values and what we are able to see here is that for a given slope and an intercept with the equation that are set as mx + c were able to generate the values and you should be able to plot them very easily.

So when you say plot x, y beautifully get a straight line. And the most important thing here is that you do not see the number the data that you have generated so one way of doing this is by giving a comma with a quote o which says that it will show the points in here. And if you would like to join the points with the line you can give something like this where you are able to see these are the points that I have generated and these line indicate direct connection between these points that have been generated.

This is not a fit in by any mean. So one has to one should not confused himself or herself with it. The advantage right now is that if you are able to change if you would like to check how this slope for -5 works out you can give this value backup and of course you have to type hold on to the plot to remind and then I can repeat y = mx + c and I can say plot once again x, y, o dash this type we will say red color, o s so that we can distinguish from what we got.

And then if we take a look at the figure what you are able to see is that the same one but just at the slope has been changed with no change whatsoever at in the intercept ok. So what we are able to realize in this is that with a mere change of a variable you can generate another set of numbers. Once again the reason for simulating something as simple as this is so that you understand how variable will work. And how numbers can be generated once you know a given function ok.

Now this is done you wanted to understand how numbers can be generated when you have multiple sets of m’s and c’s. So let us try to do the same thing I have already written a code here where I will go stepwise here. So what are we doing so we start with we are clearing all the variables and then you are clearing the screens so that you do not end up seeing lot of numbers that you might not want to see right now.

And then you are declaring the variable x that goes between 0 and 10 with 1 integer units let say between we can actually say -10 to + 10 with 1 integer units. We are giving a certain set of slopes so we call it m1 which is 5. So we are giving m1 that is 5, we can give m2 as 6 or even -5 that what we just simulated. And then we can give different sets of slope. So we can give c1 as a what did we give just a moment back we give c1 as -2.

And just for the sake of simplicity we can give c2 as also -2 because you also want to generate with the same set of numbers ok. Now that is done now you have to end up doing is to say y1 is m1 star x + c1 and y2 is m2 star x + c2 and then you can always say plot x, y1 with a o dash and hold on this indicates that the figure will not change anything there. It will remain the old set of data that you have just plotted and then plots the next set of variable.

And then you can always give an x label y label. I have just shown you a moment instead of typing everything in the command line here you can type as script out of this and then just go here and say run. When you run what you are able to see of course this time we have plotted between -10 and + 10 and you may generated x between -10 and + 10 and what you are able to realize that the intercept is exactly the same well the slopes are same in magnitude but opposite in sign. And therefore you get something like this.

And also what you are able to realize is that x variable x label and y label are also been given where the x label here is an independent variable well y is a dependent variable on x ok. So the advantage of doing this right now is that we can quickly change things slope instead of giving -2 we can also give a +10. And let see how the curve looks now accurate able to realize is that the value 0 well this has a the blue curve has a value -2 while the blue curve has the value -2 the red one has a value + 10.

In fact this is what you have given for the blue you have given a intercept of -2 for the for red you have given the intercept of + 10. So what you are able to realize is that you can quickly change this. But of course, this is also laborious because you need to keep on defining what is your m? And what is your c? So what you will see in the moment is of how to generate this quickly on the flow.

So one way of doing this is that you can once again create x variable to a start with it is better to clear any variables that you had or otherwise MATLAB can get confused or rather you might confuse MATLAB in the way you define so -10 1 integer unit until 10. Instead of giving slopes this way you can give a slope which is also n array we can also give intercept that is an array which we had just ended up using.

So far what you have seen we are declaring the variable x and we also declaring the variable m and then we are declare declaring the intercept as variable c. Now this has been being done so let us define in this program once again I am restarting it by clc which means that I am clearing the screen and then clearing all the variable and defining x between -10 to + 10 with 1 degree increments.

And let us try to give slope as 5 and -5 and then we can give intercept as -2 and +10. After having done that we are defining a variable y which will be a final answer. Let us not worry about it right now. And then what we are trying to do what we are trying to do here is to loop it across the different length of m and c meaning that now if you define m as 5, -5 and then if you ask the query what is the length of m? It says length of m is 2.

For instance, let say we define m with the 3 variables and if say m is going to find what is the length? So similar can be done for length of c. So if you are able to realize we defined 1 / 2 matrix so saying the length is 2 meaning that it takes the larger of 1 and 2 and just its 2 is the length. So what am I trying to do here is that we are trying to loop it over. So let us once again take a simpler example let us define x between -10 and +10 and then we can define m as -5 + 5 and -5.

Since we have defined these 2 what one could do here is that we can try to say for i which is an incremental variable let say going from 1 to the length of m before going there we will ask what is the length of m? Length of m is 2 we can say for i going from 1 to length of m give me y = mi star x. So now if you say y what you are able to realize is that y has been done 2 times probably and then it comes up in a way that the second variable.

If you realize the slope is -5 the values will keep reducing when you say plot x, y will be able to see the second plot that has come up ok. That is the new line that has come up it is parallel to this because we have not set up slope which is why it passes through 0, 0 and in a previous case it pass through 0, 10 right. So now what we are realized is that although we have 2 different slopes we are not able to simulate both.

So one way of doing this is once again going from let us say y of I = m of i star x and so now if size of y you are able to see both has been calculated. So let us try to see whether whatever we did made sense there you go. So you are able to plot it but of course here the intercept is 0 for both the cases which we are not very happy with. But what you are able to realize is that when we declare a variable x and m you can calculate y while looping through different values of x.

Unlike the last time where we have to keep on repeating writing the formula all that you did here was to write the formula once. But remember if you are trying to vary m and x as different values in which case let us say if you are varying m 2 times and c 2 times and if you want to find out combination of m and c the you have to repeat the formula 4 times. But here you do not have to really do that. And you can also have varying lengths of m and c such that this can be easily generated.

So now what we are trying to do here is that we are defining a for the first loop as the incrementing variable i. So whenever you say for i = 1 colon length of m and let say what is the length of m? See the length of m is 2 in this case. What it does is that its i value is 1 to start with and then goes into this portion of the code where it is once again ask what is the variable of j and to start with j is also set to 1 and it is asked what is the length of c. Length of c is also 2 so it starts with i = 1, j = 1. Then it goes here and calculates for that given values of m which is m of i and c of j.

So it can do every combination of m and every combination of c in this code. After it does that it plots it keeps the graph on and it sets it to a new variable called y and then it goes and increments the value of i from 1 to 2 because you have the length of m is 2. Then what ends up happening i becomes 2 and then it gets in to this loop and it sets that j = 1 and j = 2 and calculates all the 4. So one thing that you can do right now is that we can execute this code instead of typing each of the command at the terminal that I have written the code in a simple script and when you hit run what end up happening it also ends up plotting the figure for it.

So what has just happened here it is plotted of course with the different colors. We have not defined what each color is let actually close this and restart this. So what ends up happening is that for 2 different values of m which is +5 which are these 2 curves which are parallel to each other and -5 which are these 2 sign and purple plot which have a slope of -5 the green and the red have +5 as the slope. And of course the intercept is different for all of this for one of one set the intercept is -2. Where the red and sign meet although they are different slopes they intercept the same.

And the green and the purple of the same intercept of 10. So what your effectively done is that your massively parallelize the code such that you can generate these numbers quite easily. So that you can take a look at how do these functions looks. Of course, we have taken a very simple example nothing simple will exist in science. Therefore we will slowly complicate our life I am going to go back to make you understand how rate kinetics data can also be simulated.

So let us start with something simple we are just generated linear plots which will be can be taught about 0 order reactions. So why do not we generate the data for the first order a rate plots. Once again why are we doing this? One can always synthetically come up with data so that you can understand how to fit and we will soon see in the next part of this lecture how simulations help you come up with inform judgments of how sampling of data can be done smartly?

So that is the whole purpose of us doing this. So we are using MATLAB in this case so that you can massively paralyze or come up with numbers that can be quickly and easily generated. As always anything that starts with the percentage in MATLAB indicates the comment. So you can always add more comments to it. Comments helps one understand what the code provides. Remember this has to be put in by the coder.

Basically if the coder does not give comments you are not going to understand what it is written for. As always you start with clearing screen and clearing any variable that might exist. Remember you might have define some of the variable earlier which you should do not want or might interfere with your simulation. So it is always the better idea to for you to clear it up before starting ok. Now that we have cleared the screen and cleared the variables let us try to set the initial concentration of the chemical that you are set to 1 unit.

So it is always once again a good idea to give comments so we can say units in molar ok so molar molarity ok. This is because remember whenever you are plotting concentration is function of time you would like to know what concentration unit exist on the y axis. And if you might remember for the first order reaction A at any time t is given by A naught where A naught is the initial concentration times e power -k t where k is the reaction rate constant and t is a time variable.

So similar to x variable which is the independent variable here time is the independent variable basically that is what ends up changing and you can actually simulate the curve for different rate constant right. So we can say with command time variable and this is rate constant we can say time variable in units of seconds and rate constants in units of second inverse. And rate constant in the unit of seconds inverse ok.

So now that you have done this we can actually plot A as a function of t and generates numbers. So why do not we run it? The moment you run you get 2 beautiful curves here and remember what you can also see here you can also insert legend alright and what are you are able to see in this is that you are having data 1 that is plotted in blue which has a rate constant of 0.5 second inverse.

The data that has plotted at red which has a rate constant of 0.1 second inverse. These 2 what you are able to realize is that anything that has a higher rate constant tends to decay much faster ok. One can always add x label time in seconds so now time in second comes up then you can say y label concentration of reactants in molarity so here you start getting this and also you can all edit the labels that you have gotten by changing k = 0.5 second inverse.

This can also be coded in but I am just writing it in so that people who would like to use G Y can also use it graphical user interface and also use it. So what you are able to realize is that you are able to plot this very nicely and you are able to also appreciate the fact that are anything higher rate constant decays faster for the same time interval right. All the time point that are generated are the same for both the curves and what you are able to realize is that something with the rate constant of 0.5 falls faster and that of rate constant of 0.1.

Once again why are we doing this? We are doing this so as to understand how far or how fast can something happen so that we appreciate which variables in the function that you are looking at make a huge difference ok. So now that you have done this what we are done so far? We have been able to simulate very simple numbers with MATLAB by using linspace or other commands. And we were been able to draw plotters straight line by stimulating a straight line and then we are also been able to change the slope and intercept quite a bit in different pace and do all possible combinations of slopes and intercept and plot them.

And we have also done non-linear plots which as an exponential equation that goes here. One can also try to see whether the lon plot work out. So you can also say lon of A so MATLAB does not like ln so log, log stands for natural logarithms in MATLAB and then you have what is your to plot is that you have to plot log of A function of t can also plot so we can say if we figure 2 plot time as a function of lon of A. So let us take a look at figure 2.

So you are what you are able to realize so we are not able to see the dot so one good way of doing this what you are able to realize is that lon as a function of t comes out beautifully as a straight lines. So once again any equation that one is able to get in any form it is a good idea to numerically simulate it so as to understand which variable affect in a way that can be measured quantitatively.

That is the whole purpose of this course is not it? So what you are able to realize is that these code can also be put back in so that I can write lon of A next time this also gets done automatically. So what has happening you have 2 figures, figure 1 that shows A as a function of t the other one that says lon A as a function of t. So you can close this as well and we can start adding even more details to these plots so as to make your life easy. So you can say x label time in time in seconds y label A n molarity.

And then you can say grid on so as to even say a grid on it and then you can do the same thing here. So time in seconds lon of A remember lon A will have no unit because log of any number does not have any units. So when you run it you are able to see everything that goes here. And of course you can always insert many things can insert the title for given curve saying concentration of reactants as a function of time first order kinetics right.

So you are able to add lot more things that you like to add. So if you see here you also have the legend that we can add so that legend also says how it goes colorbar can be added in this case. Colorbar does not make sense because we are not doing a plot that varies which shows some contours or anything that sort and you can add a line or an arrow you can try to say at this point. What is the difference that comes up and if you are able to see the large difference that come up between the 2 data points of the similar curves so we can try to say insert arrow?

So what you are able to show is also illustrate the annotate and illustrate the figure can all double edged arrow lot of things text box, rectangle, eclipse to say to pin point in a certain region what is that you are trying to see as a characteristic and many such tools. Of course you can also add other labels that go in axis which has grid line on either side. You can have other toolboxes to zoom in zoom out so that you can make a plot out of it. So let us say we zoom in their and then what you can do is to save this as an image plot where you can save it as jpeg image first order zoom in ok.

So it gets saved in the folder that you are trying to look for so let us quickly check whether it did save it. What you are able to see is that the figure that you ended up generating also can be saved as jpeg. So that this helps you to understand how the MATLAB can also generate the data that you have made I mean in this case we are simulating but you can always have the x and y variable that comes up from the data set.

If you remember the determination of critical micelle concentration for a surfactant we had an output file from the Fluorescence spectrum meter which had the wavelength that varied and intensity was the output that we got. So you can plot the intensity as a function of wavelength and you should be able to check all this points find the maximum for instance and figure out which wavelength of maximum came off. So similarly to this we can excuse me we can also do the second order rate kinetics. So it is always a good idea to start since we are having a same set of variables is always better to start.

Clearing the screen and clearing the variables and running this code and I am not going to go detail of this as time is once again between and 0 and 10 seconds one has to be careful here concentration then time in seconds and then rate constants in appropriate units. Remember this is second order rate constant so therefore it is also going to have a concentration inverse that goes in concentrate inverse, second inverse this is the kind of rate constant that you are trying to look for.

So now when that goes in you would like to generate equation of this part where you would like to have A so rather y is 1 over A naught, A naught is the initial concentration. K is the rate constant and t is the time variable then you will plot t as a function of 1 over this because remember you want to plot concentration of reactants of a function of time. Then let us quickly go and run this. So when you are able to run it let us take a look at the figure that you are obtained. So it is the good idea to close the thing that you know opened and then run the code there you go.

What you are able to realize is that unlike let us insert legend first before we start talking ok. So let simulate with the same number that we had. We had 0.5 and 0.1 so let us simulate what ends up happening here is that you are able to appreciate the fact that similar difference is coming up and may be the differences for second order or more than the first order. However we sure to say that if you have the same initial concentration let simulate all of this in this same curve ok.

So let us try to say A = A naught star exp - k star t exp is that it is exp so this is first order second order ok. And then we can say plot t as a function of A which is what we suggest it but ok. Now let us run it. So what you are able to realize here is the same exact thing starts to happen we can actually make it red so that we can distinguish and make it blue and we have (()) (38:20) data close all here there you go.

So we know our fact right now that this is a second order plot for first order plot and what you are able to realize here is that anything that comes in red is the second order plot this is for 0.1 units of rate constant. This is 0.5 and same thing for 0.1 versus 0.5 but the blue one stands for the first order, the red one stands for the second order. Is that for any given point of time the second order ends up having a lesser difference between the reactants at any given point of time for different order.

So once again between 0.1 to 0.5 one can actually find the difference at any given time point and figure out what is going on. And so I think there are too many points here. So let us try to simulate with less number of points and this is what you are able to see. And let us try to see at time point of 4 so we are trying to ask what is y and actually we want what is 1 over y and we want what is A so what you are able to realize here is that this is for the set of numbers that changes a 0.5 as the rate constant.

This is 0.1 and this is for second order and this is for first order. We will see that data point the fall for the first order is much more than for the second ordered which makes no surprise because your exponential function while this is a second order polynomial. And if you remember the Taylor series the expansion the second order polynomial is just a portion of the exponential function. Exponential function also has the linear second order third order and all the other higher order that is come up.

And what ends up happening is that as the steps go forward the difference between the first step and second step is only about 0.17 units here but it is about 0.34 units here which kind of clearly indicates about 24 units here which clearly indicates at the first order falls much faster and that of the second order. So once again what this helps you to understand although you would have learnt reactions kinetic for very long time in you life.

You can easily plot this to understand what differences can come up for the same rate constant of course with different unit with same magnitude of rate constant with a given time which falls faster ok. Same thing can be done for 0 order but that is much more trivial to do I will leave it to you guys to perform the same. So let us go to the next problem then whenever you type a wrong command it actually tries to say that the function does not exist and it also suggest which function we may ended up hitting here. We hit enter it which helps you to job done faster.

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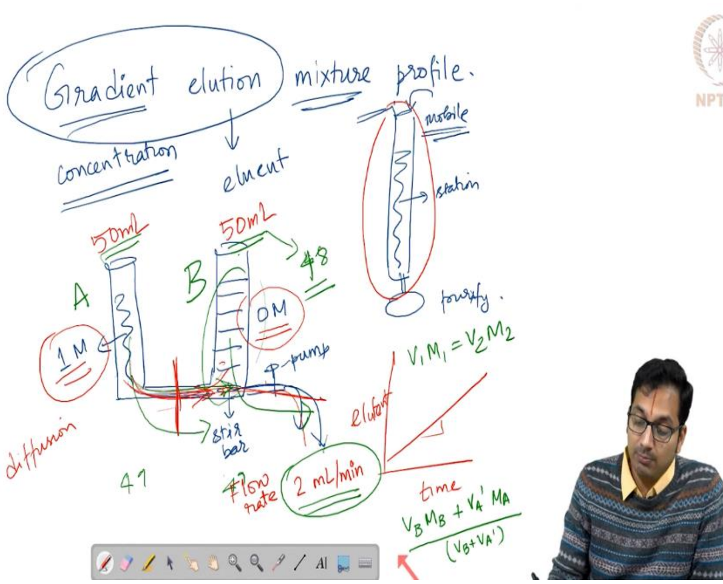

Now I am going to switch gears and try to say ok now that we have simulated different things. Why do not you simulate something that might actually be something close to real life example. And in order to do that since it is analytical chemistry course I am going to be taking up an example. The example I am taking here is to simulate a gradient elution mixture profile. What do I mean by this? What is gradient? Gradient means as a function of time something changes in this case concentration of the eluent.

You will see in the subsequent lectures in this series. What is chromatography? In that you will be using a column and the column will help you purify something will be made of column material. You will be adding a mobile face the solid material the stationary phase and then you will be adding your analyte into this and let the mobile phase help you to purify the chemical that you prepared.

Now at times the mobile phase instead of having a constant concentration might have a gradient concentration. Meaning that let say if you are doing a affinity chromatography what you would end up doing is to change the eluent concentration with the respective to something. Let say if you are doing a cation exchange column you will change this concentration of the salt as a function for time as to elute serially different chemicals that have been bond to the column.

So basically in order to do this you need to mix 2 different solutions such that the gradient elusion can be done. This is commonly done in chemistry by having a setup that looks very close to this, this goes to the column. Of course this is very simple schematic that I am trying to draw where there will be a magnetic stir bar ok. And this is the solution let say at 0 molar concentration and this is the solution at 1 molar concentration. And of course there is a pump that helps move the solution from here.

So what will end up happening since this water and these 2 are connected by connected by a tube which could exchange the liquids what will end up happening as you keep removing liquid from here as the volume across 2 of the tank should remain same there will some that flows from here to here. So when that happens what is going to end up happening you are going to mix chemicals of 2 different concentrations.

And what we are trying to do is to slowly ramp up the concentration of the eluent that goes into this chromatography column slowly such that as a function of time the concentration of something linearly increases ok. So that is the whole purpose of this. So why do not we try to take an example of course there are certain assumption that go we are assuming diffusion does not happen. Meaning that diffusion is a passive process there is a concentration gradient it will start going inside that is why you have a pump here.

Meaning that your pump keeps on sucking solution from this of course to starts with this will be closed to the barrier and only opened when the illusion is required. When such a thing is happening when the pump is removing solution from here solution will only move from here the reverse process will be less probable. And the same case what you are expecting is that the flow rate meaning the rate of which at which it is flowing the pump has enough pressure such that the back flow cannot happen.

And it matters on both side because of diffusion happens on either side this is going to get more diluted and this is going to get more concentration that will result in concentrations of the profile being quite different from whatever you wanted it to be. So therefore one has to be very careful in setting this up. But this has been quiet very well done for many decade right now. So let us take a look why do not we try to simulate this. How would we simulate this?

Let us think about it let say that there is a certain flow rate. Let say we set the flow rate what is the flow rate? Amount of liquid that comes out of this tube that are given unit of time let say the flow rate is set to 2 mL per minute. And you are having initial concentration let us say this reservoir has 50 mL of point I mean of 0 molar. This also has 50 mL a 1 molar it is quiet imperative to keep the volume constant because the volumes are in constant water is going to flow from one to the other.

And if you are special have unequal volumes of flow is going to be quiet different although you have a pump here. So it always advised to have the same volume as to achieve this. So when this is going end up happening this is open this up with this given flow rate slowly solution is going to move in. So the variable that we get to alter is the flow rate and we can simulate assuming that when you take 2 ml out of this meaning that when it goes from 50 into 48. This is not the way in reality it works.

If you take 0.2 mL it is going to also get equilibrated from other tank. But for stimulation purpose is we can take the step that are equal to the flow rate. And when that happens instantaneously 2 mL flows from here to here the dilution happens. How does the dilution happen? We can use the equation V1 M1 = V2 M2. And of course this is not a straight forward equation because you have a certain volumes here. So we can say this is tank B and this is tank A. So you have a certain volume B we have certain concentration in B.

And certain amount of volume comes from A so we can say volume A prime time concentration of A right so divided by total volume of VB + VA prime. Remember when 2 mL flow rate happens it goes from 50 to 48, 1 mL this stimulation will flow from here to here. So, as to keep the volumes 49 and 49 mL respectively because water will always try to be in the equal level. So by doing this stimulation one can try to understand how long or how much can be done. So that is what we are going to be simulating.

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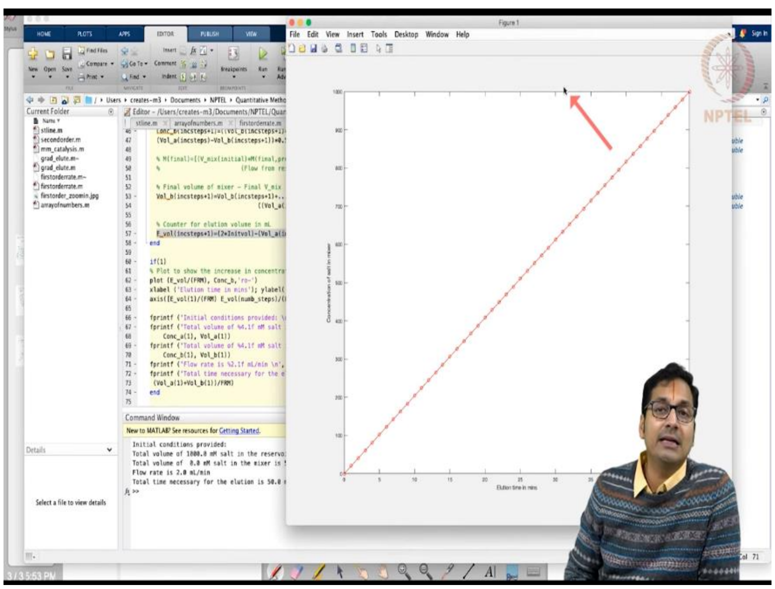

It is a very simple first order stimulation. So let me open the gradient elute stimulation and if you realize this is a stimulation that is written with a lot of inputs here or information has comments. So you will always start with a close cell so has to close any figures that have been open clear clc clear cleans up any variable in the work space and clc ends up cleaning anything in the terminal and if you see here the assumptions are also written and you are able to see a sections where initial conditions are set up.

I am putting the initial volume to 50 volume in mL and then the concentration we agreed is 1 molar. So we can write it in milli molar so we can say 1000 milli molar. So concentration in B this is where the reservoir from which the solution goes into the column and then of course we are setting the initial volume in both of the reservoirs within a given variable initial volume. And flow rate per minute which has short formed as FRM is given as 2 in this case it is 2 mL per minute.

And then I am calculating the number of steps if you are able to realize if you have 100 mL of total solution 50 mL in reservoir A 50 in B about 100 mL has to be eluted out. If 100 mL has to be eluted out what ends in happening is that if you are having 2 mL flow rate you are going to run the entire flow for about 100 mL / 2 mL per minute that is going to be 50 minutes that comes up. So just calculating it I am just trying to say the initial concentration of the eluent is 0 molar concentration of eluent in molarity.

Then similar way that we did last time we are calculating the number of increments steps such that number of steps in this case we would be having 2 mL flow rate 100 mL is going to be a going to calculate a 50 number of steps. And then all I am doing here is carefully doing each step that I have mentioned. The first step here is to change the volume from reservoir B where I say volume in reservoir B in the next step is going to be the volume that was there previously minus the flow rate.

Meaning that if you started from 50 mL if you are having 2 mL per minute if your assuming that is your quantum you are trying to simulate if you to take 2 mL out of 50 mL it is going to be 48 ml. And after having done that you should also calculate the amount of volume that will come up from A into B and how we are calculating this? The volume in a reservoir A after the change is going to be a initial volume in this case it will be 50. And the volume that you are just calculated which is 48 and that divided by 2.

So you are going to have 50 + 48 / 2 which is going to 49 just doing it in first point so that they can understand better. So now what is going to happen you are going to have 48 mL in reservoir B and 49 mL in reservoir so basically 1 mL is going to flow in. If you take a little bit of time where the comment also give you here how the equation is calculated you will understand it said that the concentration of B in the next step has to be volume in B VB times MB + volume A -

volume B basically 49 - 48 how much flows in times half of it time concentration of A divided total volume that you are calculated in A.

So basically this is the formula that I just wrote here in a very quick fashion basically you want to understand how much is in volume in B what is the concentration in B? How much volume flows from A and what is the concentration of A? And then the total volume that ends up coming which is after equilibration it is 49 mL. After having done that you want an increment of the volume. So 1 mL is added in volume in the reservoir B so 48 become 49 and then you are calculating the concentration of the eluent and then the next step you are doing is plotted.

So why do not we quickly run this simulation. So what you are able to realize is that the concentration that comes out of the elusion assuming no deification all the other assumption that are gone as a function of time if you able to realize it goes from 0 to 50 minutes. Let me make this little bigger it goes from 0 minutes to 50 minutes and in the elusion time it has nicely have a linear gradient that comes out of it right.

So what you are able to realize is that any set up that you might end up doing you would be able to simulate things in a nice fashion. So as to ensure that whatever you are thinking is what transpires when you are actually making the setup ok. So simulation are an extremely wonderful tool for one person to understand how this is the system going to behave provided you already have a model exist.

For instance we are trying to talk about how free energy changes the function of temperatures one can easily plotted right. If you know the equilibrium constant as a function of temperature you could actually calculate what is the delta G naught because it is given by delta and G naught is -RT lon of k. You know the value of k, you know the value of T you should be able to do this right. In the next lecture that we will be seeing in we will be trying to understand how to simulates such rate kinetic. And I will taking Michaelis Menten rate kinetic for that as an example. So that we understand how this works out thank you.