Dealing with Materials Data
Collection, Analysis and Interpretation
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Lecture 10
R as calculator and plotter: Diffusivity, scaled temperature

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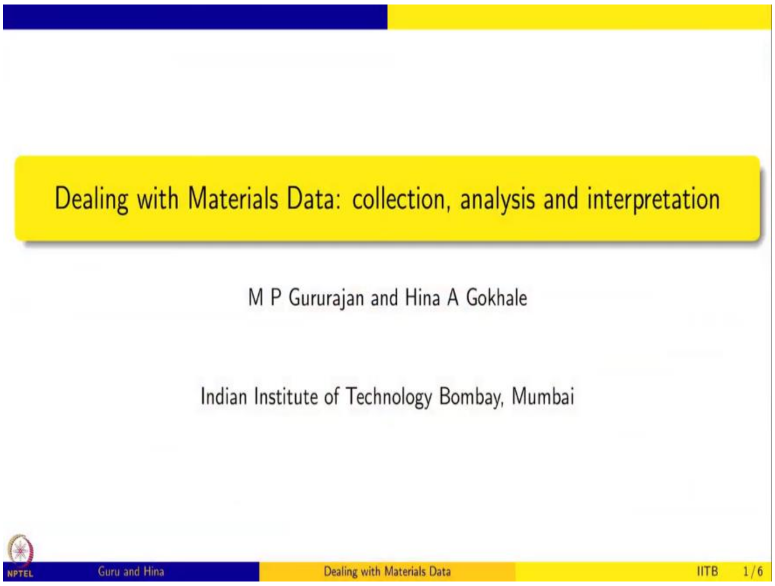

Dealing with Materials Data: collection, analysis and interpretation

M P Gururajan and Hina A Gokhale

Indian Institute of Technology Bombay, Mumbai

Welcome, this is the course on Dealing with Materials Data, we are going to discuss the collection, analysis and interpretation and we are using R to do this data analysis.

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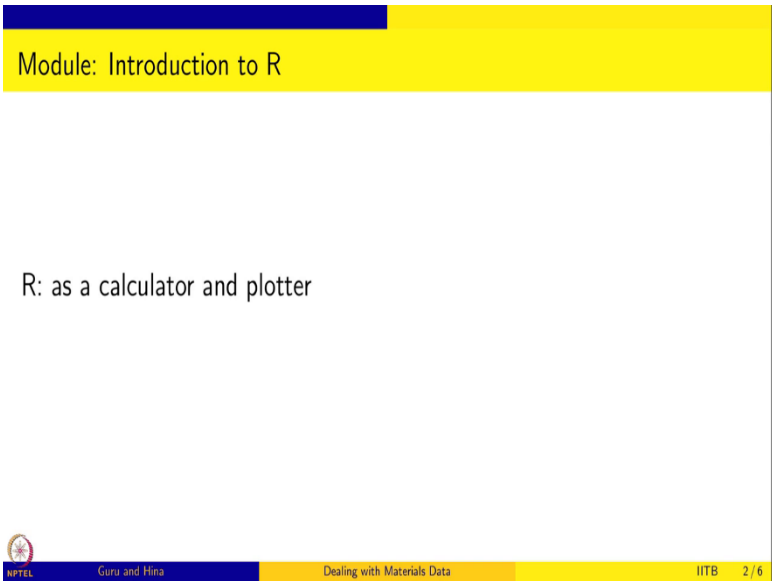

Module: Introduction to R

R: as a calculator and plotter

In this section we are going to use R as a calculator and plotter. So, we are going to use R for understanding data, how to plot data, how to interpret data and so on and so forth. But before we do all that I just want to show you that R can be used simply as a calculator and plotter. So, we will take some specific examples from simple material science and engineering and try to use R to do some calculations and plotting.

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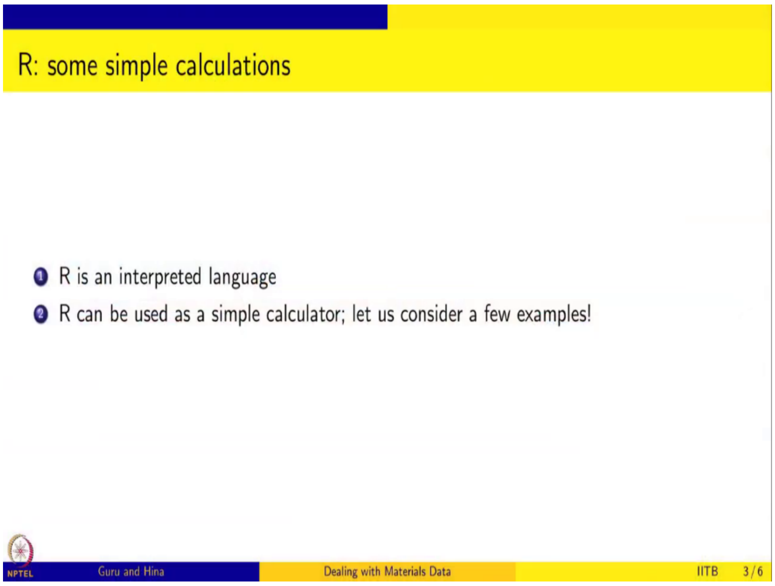

R: some simple calculations

1. R is an interpreted language
2. R can be used as a simple calculator; let us consider a few examples!

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So, like I mentioned earlier, R is an interpreted language and so, you can use it exactly like a calculator, you type in some computation and you will immediately get the answer. And so, here are a couple of examples that I want to do.

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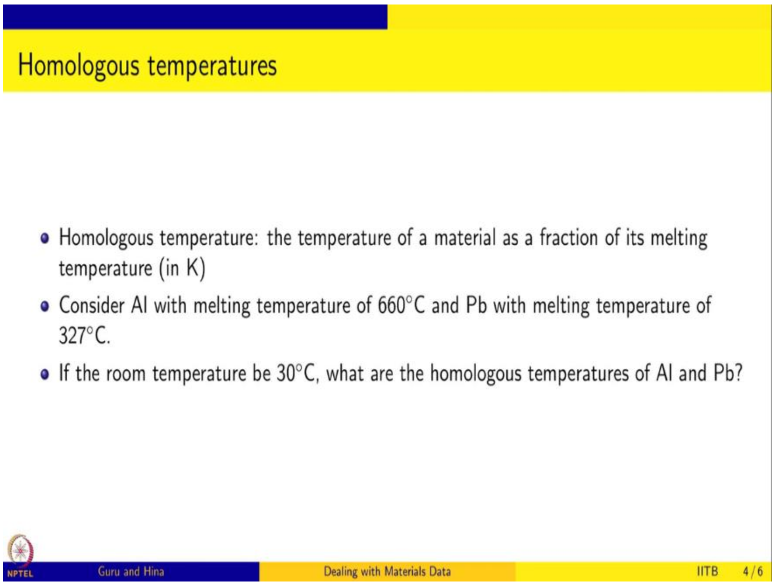

Homologous temperatures

- Homologous temperature: the temperature of a material as a fraction of its melting temperature (in K)
- Consider Al with melting temperature of 660°C and Pb with melting temperature of 327°C.
- If the room temperature be 30°C, what are the homologous temperatures of Al and Pb?

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Homologous temperature is a concept. So, it is a temperature of a material as a fraction of its melting temperature and homologues temperature is a fraction of the temperature of material as a fraction of its melting temperature in kelvin. So, if you know the melting temperature of a material in kelvin, and then any temperature of interest, if you keep that material, what homologues temperature that corresponds to basically what we are saying is at homologues temperature is a way of normalizing for the melting temperatures so, otherwise it becomes difficult to interpret results.

For example, and it is it is very funny. For example, if you take ice, if you are at minus 1 degree Celsius, where you might think that it is very cold, but for ice, it is very high temperature right, low temperature for ice might be minus 20 or minus 40 or something like that.

So, we want to get rid of this dependence on where the melting temperature is. So, in Kelvin scale, so, everything is positive. And we are going to say the given temperature divided by the melting temperature of the material, then you can compare different materials for example, a Homologous if temperature is 0.5 for two different materials, then both of them are at a temperature which is 50 percent of their respective melting temperatures right. So this concept is very useful. So let us say that we want to calculate the homologous temperature.

Let us consider aluminium which has a melting temperature of 660 degrees Celsius and lead which has a melting temperature of 327 degrees Celsius. And let us say both of them are at room temperature. And let us assume that the room temperature is 30 degrees Celsius. What are the homologous temperatures of aluminium and lead? So this is what we want to do.

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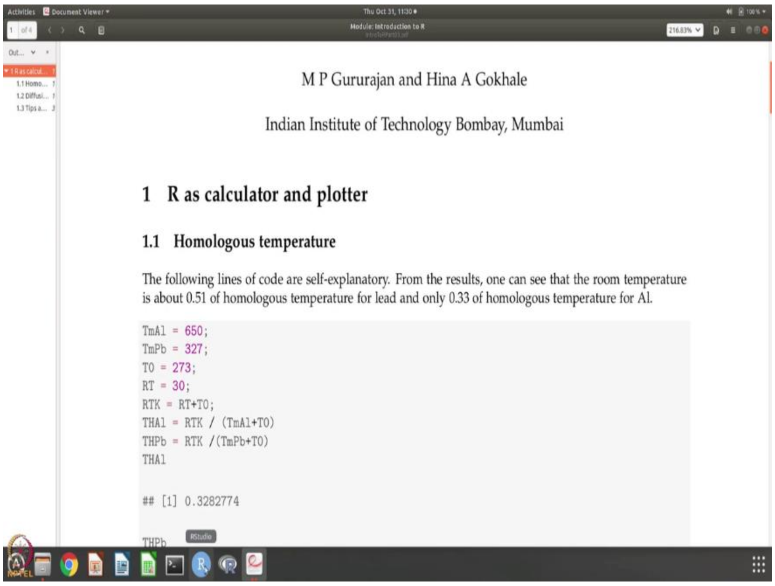

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1 R as calculator and plotter

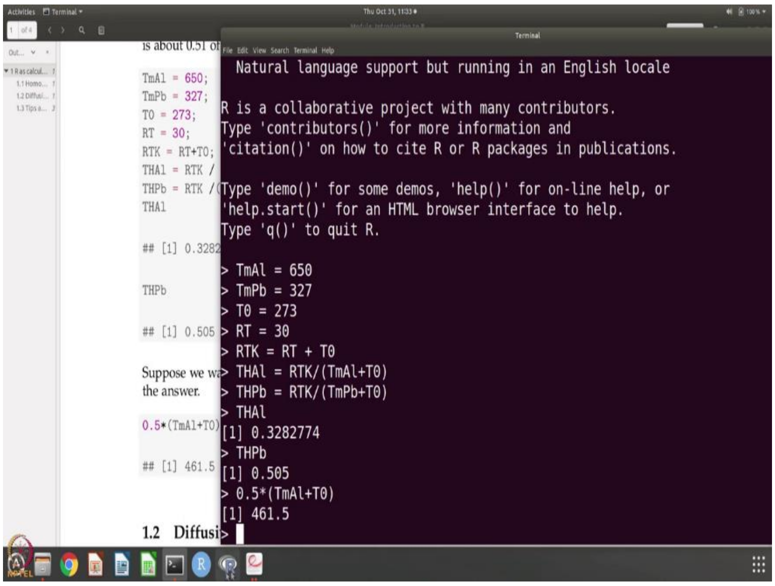
1.1 Homologous temperature

The following lines of code are self-explanatory. From the results, one can see that the room temperature is about 0.51 of homologous temperature for lead and only 0.33 of homologous temperature for Al.

```
TmAl = 650;
TmPb = 327;
T0 = 273;
RT = 30;
RTK = RT+T0;
THAl = RTK / (TmAl+T0)
THPb = RTK /(TmPb+T0)
THAl

## [1] 0.3282774

THPb
```



```
 Natural language support but running in an English locale

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'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> TmAl = 650
> TmPb = 327
> T0 = 273
> RT = 30
> RTK = RT + T0
> THAl = RTK/(TmAl+T0)
> THPb = RTK/(TmPb+T0)
> THAl
[1] 0.3282774
> THPb
[1] 0.505
> 0.5*(TmAl+T0)
[1] 461.5
> 
```

Like I said, we have the notes, so this is the notes and notes and notes gives you all these commands, but I am also going to type it so that you can work with me. Let us say that temperature of melting for aluminium is equal to 650. Temperature of melting for lead is equal to 327. So you might see in my notes that I have this colon so this is habit from writing scripts in active but it is not essential so you do not have to put the colons.

And the room temperature and so we need to transform all these temperatures which are in degrees Celsius to Kelvin. So I am going to add a 273 to them so T^0 is 273. And I am going to call this room temperature that is 30. And the so let us calculate the homologous temperature for aluminium, which is nothing but before that room temperature in Kelvin is nothing but room temperature plus T^0.

Now, the homologous temperature for aluminium is nothing but so, melting temperature of aluminium and we need to convert it into Kelvin and melting temperature, the homologues temperature for lead is the same thing so, I can actually do this I can use the up key to get the previous command and modify it. So, it just needs these two modifications. So homologues temperature of lead is nothing but room temperature in Kelvin divided by the melting temperature of lead in Kelvin.

So now we want to know what is the homologous temperature of aluminium. It is 0.33. And what is lead? Assuming that we are at room temperature and room temperature is 30, for aluminium it is 0.33 and for lead we are already above 0.5 right and that is what is shown here.

Now suppose you want to calculate the temperature, which is 0.5 homologous for aluminium. It is rather simple. So you multiply by the so, 461.5 right? So that is the homologous temperature for aluminium 0.5 homologous temperature for aluminium. So this is the first example, so we are just using it like a calculator except that it is a more advanced calculator in the sense that you are giving variable names and you can deal with these variable names. And whenever you want the answer you can just ask for the computer and for R to give you the values and it will give you those values.

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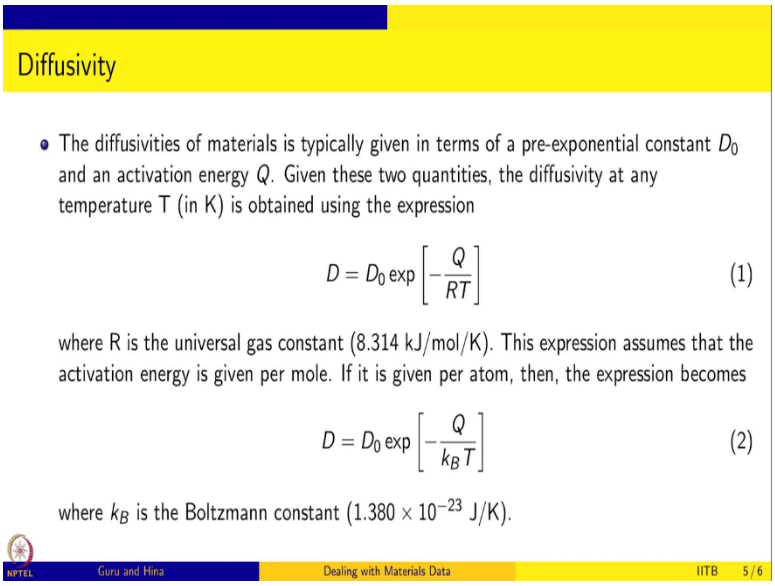

Diffusivity

- The diffusivities of materials is typically given in terms of a pre-exponential constant D_0 and an activation energy Q. Given these two quantities, the diffusivity at any temperature T (in K) is obtained using the expression

$$D = D_0 \exp\left[-\frac{Q}{RT}\right] \quad (1)$$

where R is the universal gas constant (8.314 kJ/mol/K). This expression assumes that the activation energy is given per mole. If it is given per atom, then, the expression becomes

$$D = D_0 \exp\left[-\frac{Q}{k_B T}\right] \quad (2)$$

where k_B is the Boltzmann constant (1.380×10^{-23} J/K).

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The second problem, so I said that it is both calculator and plotter. So let us take another problem. This is a problem on diffusivity, diffusivity of materials is typically given in terms of the pre exponential constant D0 and the activation energy Q. The expression of diffusivities is

$$D = D0 * \exp[-\frac{Q}{RT}]$$

R is the universal gas constant which is 8.314 joules per mole per kelvin. We are assuming that this Q is given per mole, but if it is given per atom this will just become k_B T, where k_B is the Boltzmann constant 1.38 X 10^{-27} joule kelvin. So, this is the diffusivity and so typically values of D naught and Q are tabulated and then for any temperature then you can calculate diffusivity.

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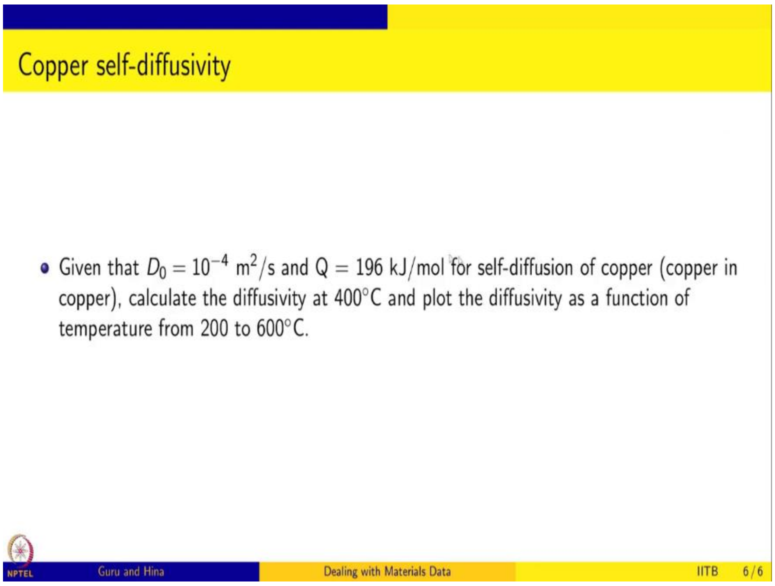

Copper self-diffusivity

- Given that $D_0 = 10^{-4}$ m^2/s and Q = 196 kJ/mol for self-diffusion of copper (copper in copper), calculate the diffusivity at 400°C and plot the diffusivity as a function of temperature from 200 to 600°C.

Let us take a particular system. So, this is copper, this is for self-diffusion of copper that is copper diffusing in copper itself. The D0 is known to be 10 power minus 4 meter square per second, and Q is 196 kilojoules. And so let us say we want to calculate the diffusivity at 400 degrees Celsius and also plot the diffusivity as a function of temperature from 200 to 600 degrees C.

So, we want to do two things, one is that given these values you can calculate diffusivity. So, this is just a continuation of the previous problem, you can use R as a calculator, you can just put these values and then evaluate the value at 400 so you will get that. And you can also plot diffusivity because we said R can also be a plotter. Plotting means we have to have a table, we have to have temperature from 200 to 600.

And for each temperature corresponding to 200 for example, 250 for example, 300 for example, and so on, you also have to get the diffusivity once you have this table of temperature versus diffusivity, then you can plot it as usual, so that is what we want to do next and so here is my notes, so this is the diffusivity problem so let us start doing it.

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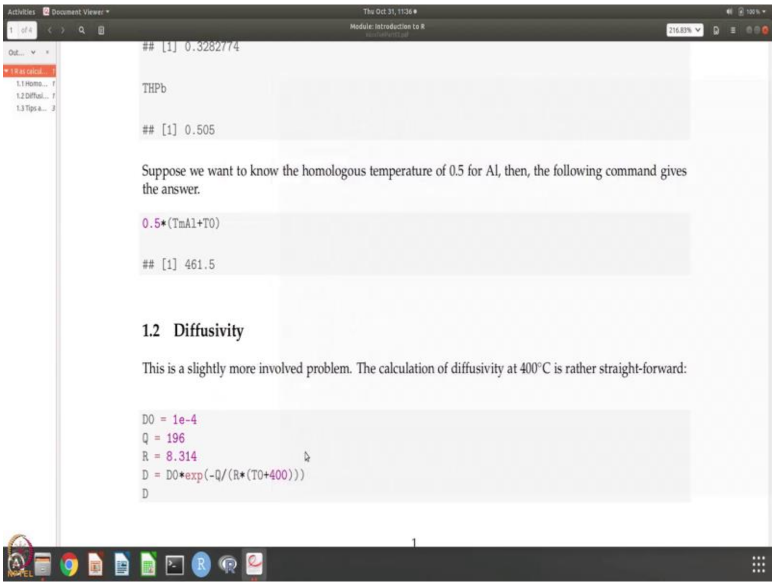


```
## [1] 0.3282774

THPb

## [1] 0.505
```

Suppose we want to know the homologous temperature of 0.5 for Al, then, the following command gives the answer.

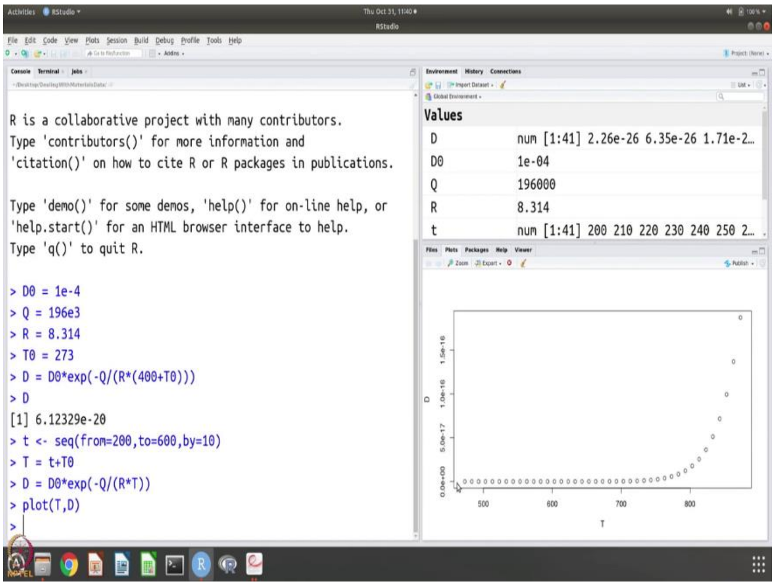
```
0.5*(TmAl+T0)

## [1] 461.5
```

1.2 Diffusivity

This is a slightly more involved problem. The calculation of diffusivity at 400°C is rather straight-forward:

```
D0 = 1e-4
Q = 196
R = 8.314
D = D0*exp(-Q/(R*(T0+400)))
D
```



```
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Type 'q()' to quit R.

> D0 = 1e-4
> Q = 196e3
> R = 8.314
> T0 = 273
> D = D0*exp(-Q/(R*(400+T0)))
> D
[1] 6.12329e-20
> t <- seq(from=200,to=600,by=10)
> T = t+T0
> D = D0*exp(-Q/(R*T))
> plot(T,D)
>
```

```
Values
D     num [1:41] 2.26e-26 6.35e-26 1.71e-2…
D0    1e-04
Q     196000
R     8.314
t     num [1:41] 200 210 220 230 240 250 2…
```

So, and this problem I want to do in the, R studio because then it is easy to see the see the plots. So what do we want to do? We know that D0 is nothing but and Q is given to be 196 remember this is kilojoules so I am going to make it joule by multiplying e power 3 and then R is 8.314.

So we wanted to calculate D at 400, but remember we need to turn it into Kelvin because temperature is in Kelvin. So D is nothing but D0 into exponential, so this is another advantage with R studio so, we did not know whether there is a command called exp but you know, it is there and if you go there, it even gives you the information.

Log computes logarithms by default natural logarithms and, and so on. Okay, so, so you have the information about exponential so this is D exp minus Q by RT, R into T is 400 we wanted to calculate and T naught. So I do not know if it is visible to you, but if I take the cursor here it highlights here, if I take the next one it highlights here and if I take next one it highlights here, so all the parentheses are complete.

So, you can calculate and as you can see, you know the values what are the variables we have defined and what their values are. So, even without printing D here I can already see that it is 6.1 10 power minus 20. So it has already come but of course, you can just say D and then it will give you that answer. But R studio environment is nice because as we are doing, you can see what is happening.

Now we want to plot for plotting, we want to get the temperatures from 200 to 600. So I am going to do let us say temperature and we want to increase let say 10 degrees. Now, capital T we want which is nothing but this t plus T0. So, as you can see, t is temperature 10 to 20, etc. And then capital T already made it into Kelvin 473, 483, 493, etc. Once we have it so we can calculate D, which is nothing but D0 into exponential minus Q by R T.

And, so let us calculate D so it is available so the D values are given. Now what do we do? We say plot T versus D and here is a plot, so you can see that the diffusivity of course it exponentially increases with increasing temperature because it is minus 1 by T. So as you can see that 400 to 800, 473 to 873 Kelvin, 200 to 600 degrees Celsius, the self-diffusivity of copper, this is how it looks.

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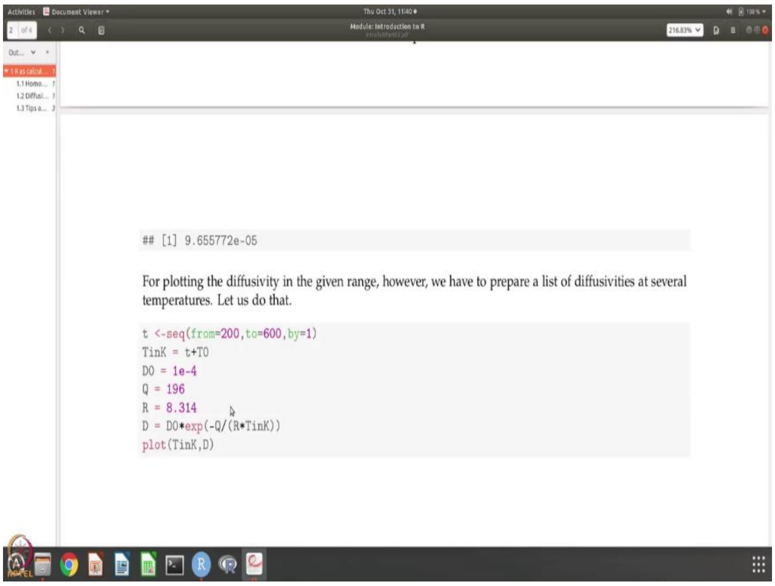

```
## [1] 9.655772e-05
```

For plotting the diffusivity in the given range, however, we have to prepare a list of diffusivities at several temperatures. Let us do that.

```
t <-seq(from=200,to=600,by=1)
TinK = t+T0
D0 = 1e-4
Q = 196
R = 8.314
D = D0*exp(-Q/(R*TinK))
plot(TinK,D)
```

So by, so it is similar here and, I think there is a mistake in this we will correct it, Q should be in kilojoules so okay. So, of course, the next thing that you want to do, let us say that I want to write a small script okay.

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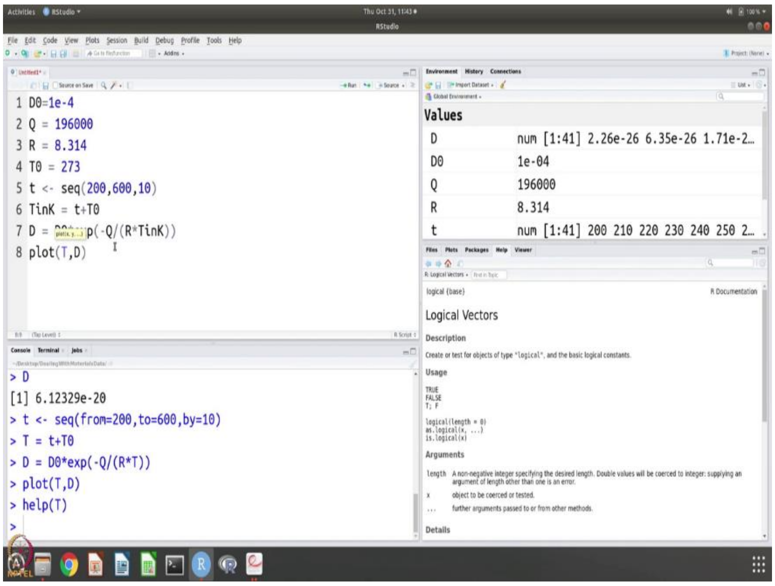


```r
D0=1e-4
Q = 196000
R = 8.314
T0 = 273
t <- seq(200,600,10)
TinK = t+T0
D = D0*exp(-Q/(R*TinK))
plot(T,D)
```

```
> D
[1] 6.12329e-20
> t <- seq(from=200,to=600,by=10)
> T = t+T0
> D = D0*exp(-Q/(R*T))
> plot(T,D)
> help(T)
>
```

Values

D	num [1:41] 2.26e-26 6.35e-26 1.71e-2…
D0	1e-04
Q	196000
R	8.314
t	num [1:41] 200 210 220 230 240 250 2…

logical {base} R Documentation

Logical Vectors

Description

Create or test for objects of type "logical", and the basic logical constants.

Usage

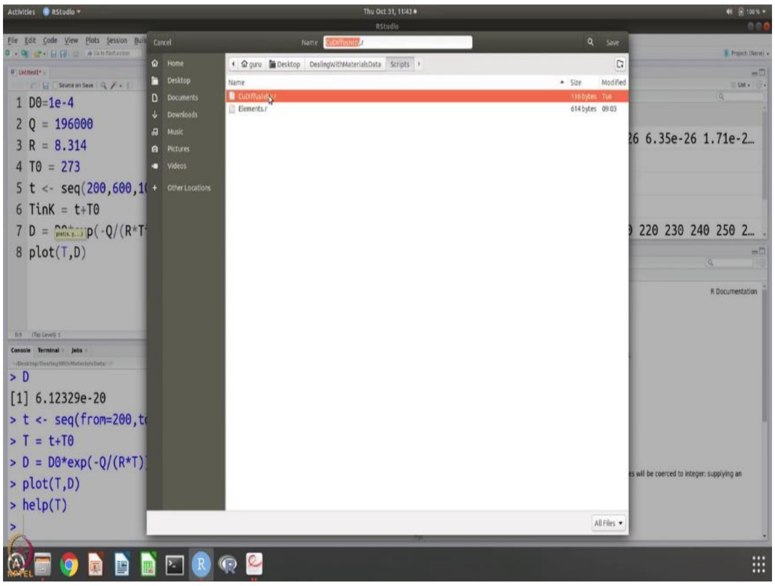
```
TRUE
FALSE
T; F

logical(length = 0)
as.logical(x, ...)
is.logical(x)
```

Arguments

length	A non-negative integer specifying the desired length. Double values will be coerced to integer: supplying an argument of length other than one is an error.
x	object to be coerced or tested.
...	further arguments passed to or from other methods.

Details



Name: CuDiffusivity.r

guru › Desktop › DealingWithMaterialsData › Scripts

Name	Size	Modified
CuDiffusivity.r	116 bytes	Tue
Elements.r	614 bytes	09:03

And what is a script is going to be, so I am going to say D0 equal to 1 e power minus 4, Q is equal to 196 kilojoules and R is equal to 8.314, and then we can repeat the rest of the commands exactly as here D0 is equal to 273 and t is equal to 200 to 600 and 10, and capital T. Now, you see when I type capital T it highlights in a different colour. That is because for true and false there are logical values so, the T is already right, true and false are represented by T and they have so I cannot use capital T, so I am going to say T in K. T in K is nothing but T plus T naught.

Now we can say the diffusivity is nothing but D0 into exponential. See that is other nice thing if I open a parenthesis, it closes a parenthesis by itself by R into T in Kelvin okay. So we have calculated, then we want to say plot T, D, so now I am going to save this file, save as, and I am going to save it in scripts and let us call it as couple diffusivity.r. Yeah, replace. Now, I can run this right, this is the script. I can run this so I will get the plot.

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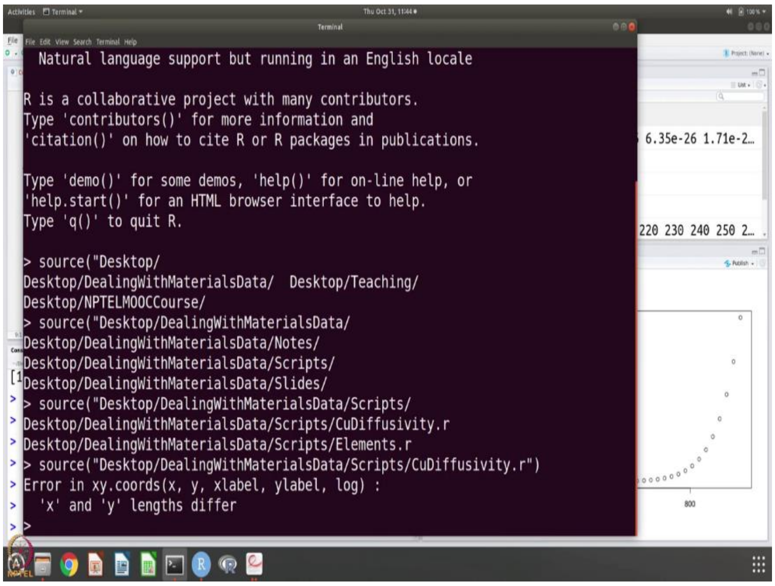

```
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'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> source("Desktop/
Desktop/DealingWithMaterialsData/  Desktop/Teaching/
Desktop/NPTELMOOCCourse/
> source("Desktop/DealingWithMaterialsData/
Desktop/DealingWithMaterialsData/Notes/
Desktop/DealingWithMaterialsData/Scripts/
Desktop/DealingWithMaterialsData/Slides/
> source("Desktop/DealingWithMaterialsData/Scripts/
Desktop/DealingWithMaterialsData/Scripts/CuDiffusivity.r
Desktop/DealingWithMaterialsData/Scripts/Elements.r
> source("Desktop/DealingWithMaterialsData/Scripts/CuDiffusivity.r")
Error in xy.coords(x, y, xlabel, ylabel, log) :
  'x' and 'y' lengths differ
>
```

There is also another way, which is to so suppose I want to run it in the R console, so I do not have this right. So I have to go to so where was this I have to look at and in materials data, scripts of diffusivity data. So you have to give the full path but the nice thing is if you know the first few letters and then press on tab, it completes, it auto-complete so you do not have to type the entire name of the directory for example.

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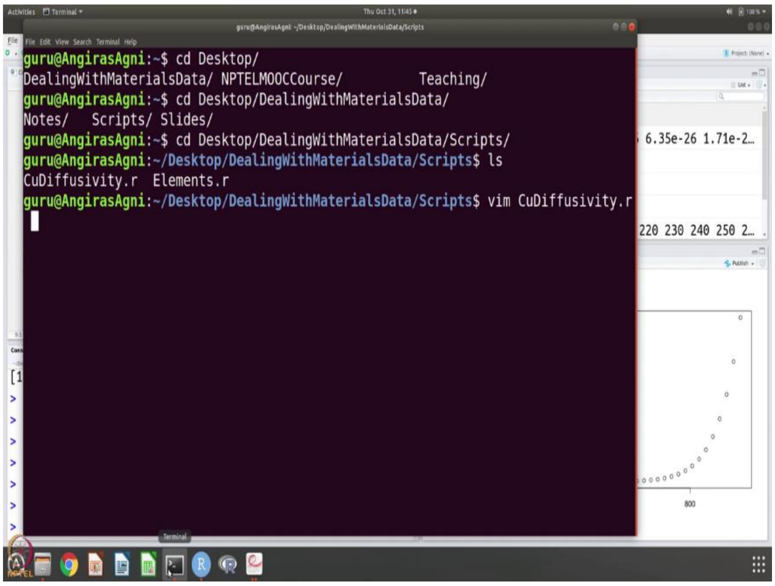
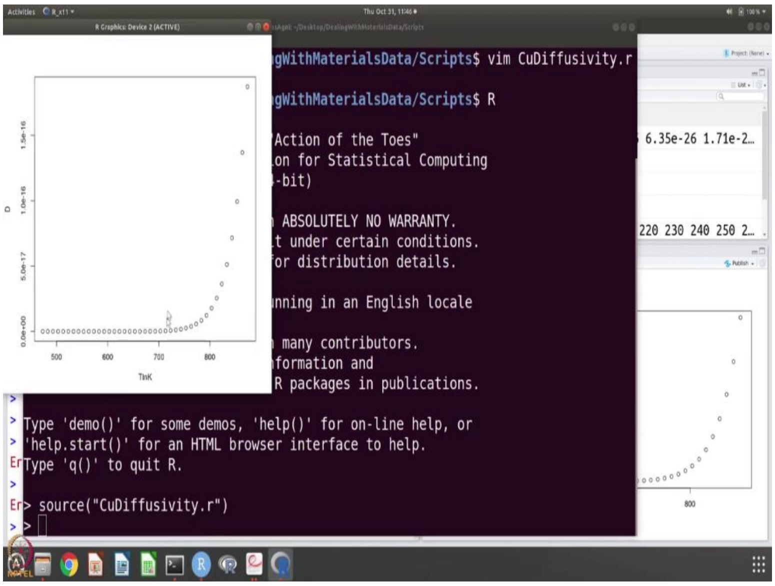


```
guru@AngirasAgni:~$ cd Desktop/
DealingWithMaterialsData/ NPTELMOOCCourse/          Teaching/
guru@AngirasAgni:~$ cd Desktop/DealingWithMaterialsData/
Notes/   Scripts/ Slides/
guru@AngirasAgni:~$ cd Desktop/DealingWithMaterialsData/Scripts/
guru@AngirasAgni:~/Desktop/DealingWithMaterialsData/Scripts$ ls
CuDiffusivity.r  Elements.r
guru@AngirasAgni:~/Desktop/DealingWithMaterialsData/Scripts$ vim CuDiffusivity.r
```



```
gWithMaterialsData/Scripts$ vim CuDiffusivity.r

gWithMaterialsData/Scripts$ R

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Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> source("CuDiffusivity.r")
>
```

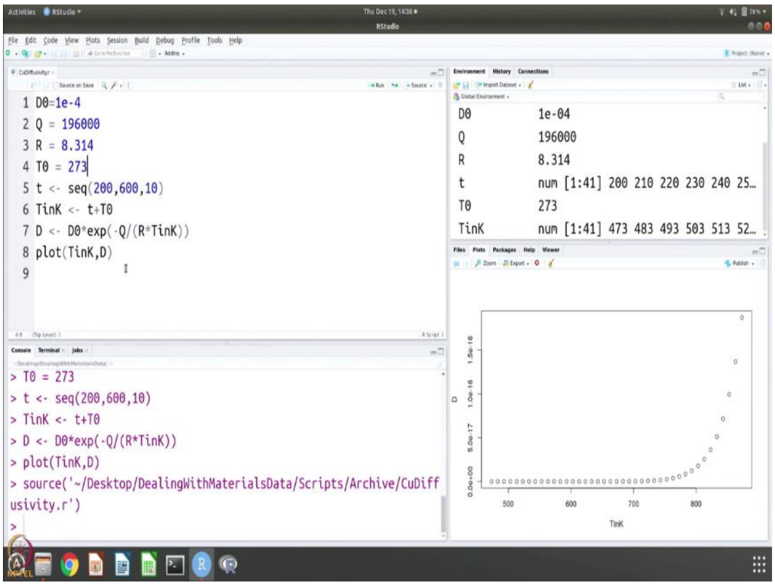

```
D0=1e-4
Q = 196000
R = 8.314
T0 = 273
t <- seq(200,600,10)
TinK <- t+T0
D <- D0*exp(-Q/(R*TinK))
plot(TinK,D)
```

```
D0          1e-04
Q           196000
R           8.314
t           num [1:41] 200 210 220 230 240 25…
T0          273
TinK        num [1:41] 473 483 493 503 513 52…
```

```
> T0 = 273
> t <- seq(200,600,10)
> TinK <- t+T0
> D <- D0*exp(-Q/(R*TinK))
> plot(TinK,D)
> source('~/Desktop/DealingWithMaterialsData/Scripts/Archive/CuDiff
usivity.r')
>
```

So if you do let us go to this, so you know what the error is. Okay, yeah, I should not have, yes save yes, so we are able to get this. And so you can also use the script and use the command source to run it. I just want to show this clarification when we were running this Cu diffusivity dot R, we did get an error message and we lost it over. I just want to show you how that error comes about and how to fix it. My cursor is on this line, D is D0 exponential minus Q by R and temperature in Kelvin. So if I just say run, as you can see, it means run the current line or selection.

So if I if I have selected something, then it would run the selection. Or if the cursor just stays there, it will just run that line. So, if I now say run it says error object D0 not found that is because we are just trying to execute this line and it does not know what the parameters are D 0 for example, it does not know or T in K it does not know things like that. So, to avoid that, you can say source and if you say source, then it sources everything which means from the first line it goes through so, you can see that the plotting is done.

So, this is something that we have noticed and when I was going back and forth between the R console and R studio. And sometimes when I was trying to execute, instead of source I used to run and because run meant just that line it gave that error. On the other hand, you can mask everything and then say run and then it will execute it.

Or you can just say source and then it will executed so either way it can be done. This is just to show you some of you might have been wondering what is that error message and why it came about so this is the reason it comes about.

So when you the source and run are close to each other. So when you do, you have to be careful as to what you are doing or if you notice error message then you know that you have been using run instead of source and so it is just running one line instead of running the entire script. So, this is just to explain why you saw some strange error messages in the session. Thank you