ENGG1811 Computing for Engineers

Week 7 (Additional Slides)

For “Example – rates of diffusion”

Example – rates of diffusion*

- Metals are hardened by *carburising*, where carbon diffuses into the heated metal at a rate D that depends on the temperature T (in K) and material characteristics:

$$D = D_0 e^{-Q/RT}$$

  - R is the ideal gas constant = 8.314 J/K/mol
  - diffusion coefficient D_0 and activation energy Q depend on the material

Material	D_0 (m^2/s)	Q (J/mol)
Ferrite (α Fe)	6.2×10^{-7}	80 000

* Moore, Example 5.3, using SI units and including some corrections

Exercise

1. Compute the diffusivity of Ferrite for 40 equally spaced temperature from 25 ° C to 1200 ° C
2. Display results on plots of diffusivity against inverse temperature $1/T$ with different scale types

Using array operations

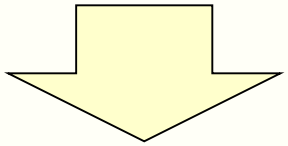
- Given the temperature vector T, how can we use the array operation to calculate

$$D = D_0 e^{-Q/RT}$$

for each value of in the vector T

- Starting point

$$\begin{bmatrix} T(1) & T(2) & T(3) \end{bmatrix}$$



$$\begin{bmatrix} D_0 e^{-\frac{Q}{RT(1)}} & D_0 e^{-\frac{Q}{RT(2)}} & D_0 e^{-\frac{Q}{RT(3)}} \end{bmatrix}$$

Matlab screenshots ...

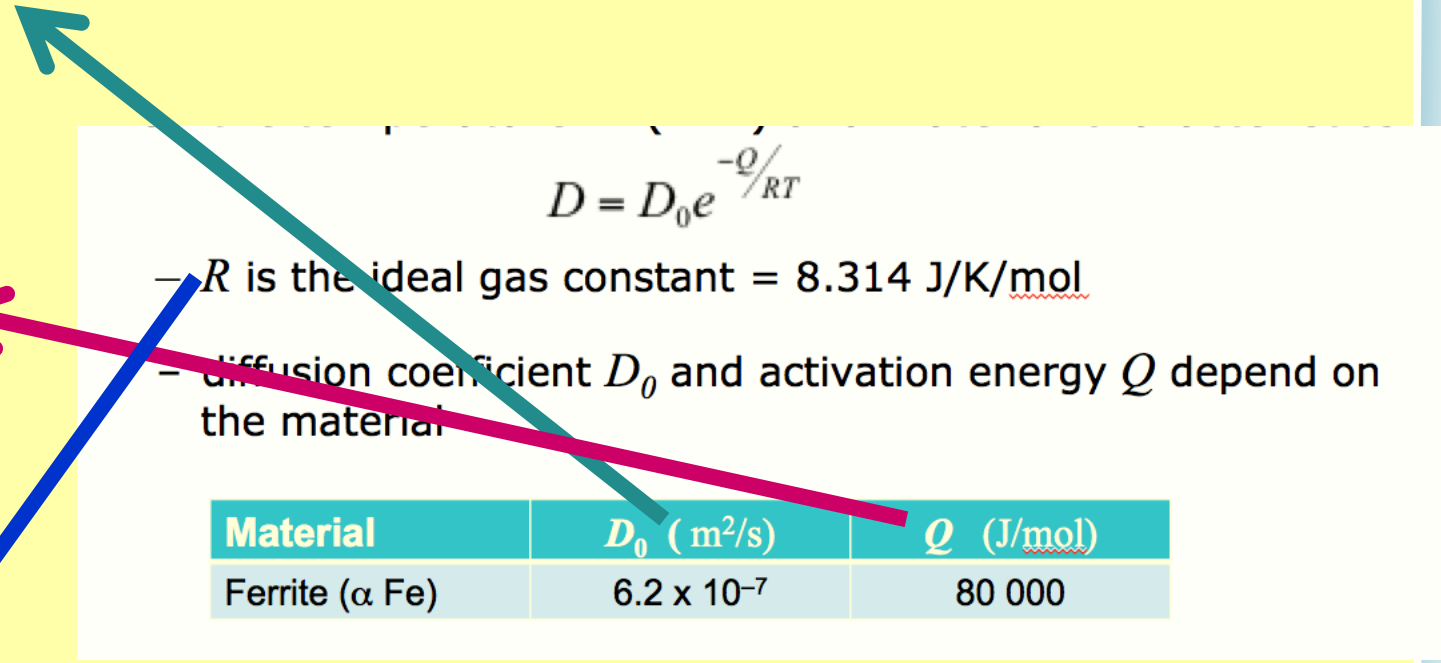
1. Compute the diffusivity of Ferrite for 40 equally spaced temperature from 25 ° C to 1200 ° C

```
>>
>> T = linspace(25,1200,40)

T =

   1.0e+03 *

  Columns 1 through 12

    0.0250    0.0551    0.0853    0.1154    0.1455    0.1756    0.2058    0.2359    0.2660    0.2962    0.3263    0.3564

  Columns 13 through 24

    0.3865    0.4167    0.4468    0.4769    0.5071    0.5372    0.5673    0.5974    0.6276    0.6577    0.6878    0.7179

  Columns 25 through 36

    0.7481    0.7782    0.8083    0.8385    0.8686    0.8987    0.9288    0.9590    0.9891    1.0192    1.0494    1.0795

  Columns 37 through 40

    1.1096    1.1397    1.1699    1.2000
```

Each value in the vector is multiplied by this

Matlab screenshots ...

```
>> Do = 6.2* 10^7

Do =

    62000000

>> Q = 80000

Q =

       80000

>> R = 8.314

R =

    8.3140
```



Matlab screenshots ...

```
>> D = Do * exp( -(Q/R) ./ T )

D =

   1.0e+04 *

  Columns 1 through 12

    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000

  Columns 13 through 24

    0.0000    0.0000    0.0000    0.0000    0.0000    0.0001    0.0003    0.0006    0.0014    0.0027    0.0052    0.0094

  Columns 25 through 36

    0.0161    0.0265    0.0419    0.0643    0.0958    0.1388    0.1965    0.2721    0.3693    0.4924    0.6457    0.8340

  Columns 37 through 40

    1.0624    1.3361    1.6606    2.0415

>>
```

$$D = D_0 e^{-Q/RT}$$

Each value in the vector is multiplied by this

Matlab screenshots ...

```
>> inverseT = 1 ./ T

inverseT =

  Columns 1 through 12

    0.0400    0.0181    0.0117    0.0087    0.0069    0.0057    0.0049    0.0042    0.0038    0.0034    0.0031    0.0028

  Columns 13 through 24

    0.0026    0.0024    0.0022    0.0021    0.0020    0.0019    0.0018    0.0017    0.0016    0.0015    0.0015    0.0014

  Columns 25 through 36

    0.0013    0.0013    0.0012    0.0012    0.0012    0.0011    0.0011    0.0010    0.0010    0.0010    0.0010    0.0009

  Columns 37 through 40

    0.0009    0.0009    0.0009    0.0008


>>
>>
>>
>>
>> plot( inverseT , D )
>>
```

Matlab screenshots ...

- If you do not want to display values, put ";" at the end of a line (see below). All we need is the following seven lines:

```
>>
>> T = linspace(25,1200,40);
>> Do = 6.2* 10^7 ;
>> Q=80000;
>> R = 8.314;
>> D = Do * exp( -(Q/R) ./ T );
>> inverseT = 1 ./ T;
>> plot(inverseT , D );
>>
>>
```

Matlab screenshots ...

- If you want more clarifications, first define T, Q, R, and Do as explained in the previous slide.

```
>> T = linspace(25,1200,40);
>> Q = 80000;
>> R = 8.314;
>> Do = 6.2* 10^7 ;
```

- After the above, try displaying intermediate values for your clarifications. Note that you do not need to do this in order to calculate D, this is just for your clarifications.

```
>>  -(Q/R) ./ T
>>
>> exp( -(Q/R) ./ T )
>>
>> Do * exp( -(Q/R) ./ T )
>>
```