Week 7 (Additional Slides)

Screenshots from Matlab (from slide 5 onwards)
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

<table>
<thead>
<tr>
<th>Material</th>
<th>$D_0$ (m²/s)</th>
<th>$Q$ (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite (α Fe)</td>
<td>$6.2 \times 10^{-7}$</td>
<td>80 000</td>
</tr>
</tbody>
</table>

* 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

$$D = D_0 e^{-\frac{Q}{RT}}$$

for each value of $T$ in the vector $T$

• Starting point

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

$$\begin{bmatrix} D_0 e^{-\frac{Q}{RT(1)}} & D_0 e^{-\frac{Q}{RT(2)}} & D_0 e^{-\frac{Q}{RT(3)}} \end{bmatrix}$$
1. Compute the diffusivity of Ferrite for 40 equally spaced temperature from 25 °C to 1200 °C

```matlab
>> 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.
\[ \text{Do} = 6.2 \times 10^7 \]

\[ \text{Do} = 62000000 \]

\[ \text{Q} = 80000 \]

\[ \text{Q} = 80000 \]

\[ \text{R} = 8.314 \]

\[ \text{R} = 8.3140 \]

\[ D = D_0 e^{\frac{-Q}{RT}} \]

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

<table>
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<tr>
<th>Material</th>
<th>( D_0 ) (m²/s)</th>
<th>( Q ) (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite (( \alpha ) Fe)</td>
<td>6.2 \times 10^{-7}</td>
<td>80000</td>
</tr>
</tbody>
</table>
```matlab
>> 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  0.0001  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

>>
```

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:

```matlab
>> 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.

\[
\begin{align*}
  & \text{>> } T = \text{linspace}(25,1200,40); \\
  & \text{>> } Q = 80000; \\
  & \text{>> } R = 8.314; \\
  & \text{>> } Do = 6.2 \times 10^7; \\
\end{align*}
\]

• 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.

\[
\begin{align*}
  & \text{>> } -\frac{Q}{R} ./ T \\
  & \text{>> } \exp\left( -\frac{Q}{R} ./ T \right) \\
  & \text{>> } Do \times \exp\left( -\frac{Q}{R} ./ T \right) \\
\end{align*}
\]
Have a Happy Long Weekend... :-}