EPSC 220: Principles of Geochemistry Laboratory 1: Introduction to Geochemical Calculations with MATLAB

**MATLAB learning objectives**
Learn how to use the following functions in MATLAB: help, roots and some of the various MATLAB functions that perform numerical integration. Learn how to write a loop for an iterative calculation and use a conditional statement to exit a loop when a solution is found (using Newton’s Method). Practice writing matrices in MATLAB and solving coupled systems of linear equations using the MATLAB backslash operator.

**Geochemical learning objectives:**
Review calculations of ΔH, ΔS, and ΔG for simple chemical reactions. Learn some geologically important reactions and the names and formulas of some end-member mineral formulas.

**Assessment:**
The goal of this assignment is to learn. If you make a mistake we will help you redo the assignment until you understand the results and obtain the correct answers.

Please feel free to ask for help and/or look up the information on the web that you need to help solve the following problems. However, you cannot simply download or “cut and paste” a program that you find on the web.

1. Measure the duration of time you need to solve the following equation for x by hand and by MATLAB (read the MATLAB help files to learn how to find the roots of polynomials):

\[3x^3 + 2x^2 + 5x - 37.2 = 0\]

Using MATLAB and the data on the next page write a short program to calculate the ΔH, ΔS, and ΔG of the following reaction at 1 bar, 298 K:

\[\text{C}_{\text{diamond}} \leftrightarrow \text{C}_{\text{graphite}}\]

2. Integrate the following equation from 1 to 100 using both numerical methods in MATLAB (see the help to find the correct command) and analytically using integration by parts:

\[\ln(x) + 3x^2 + 2x - 5 = 0\]

Using the data on the next page calculate the ΔH, ΔS, and ΔG of the following reaction at 1 bar, 298 K using MATLAB:

\[\text{NaAlSi}_3\text{O}_8_{\text{plagioclase}} \leftrightarrow \text{NaAlSi}_2\text{O}_6_{\text{clinopyroxene}} + \text{SiO}_2_{\text{quartz}}\]

3. Write your own program in MATLAB using Newton’s method to find the solution of (you will have to use a simple loop in your program):
5\ln(x) + 6\ln(x^2) - 3x + 7 = 0

Using MATLAB and the data on the next page write a short program to calculate the \(\Delta H\), \(\Delta S\), and \(\Delta G\) at 1 bar, 298 K of the following reaction:

\[
\text{Mg}_2\text{SiO}_4^{\text{olivine}} + \text{SiO}_2^{\text{quartz}} \rightleftharpoons 2 \text{MgSiO}_3^{\text{orthopyroxene}}
\]

4. Use MATLAB to find the solution to the following set of equations (remember that you can express these equations in matrix form):

\[
\begin{align*}
2x + 4y - 7z &= 0.4482643 \\
3x + 7y + 1.5z &= 31.445008 \\
x + y - z &= 2.8390049
\end{align*}
\]

Using MATLAB and the below data write a short program to calculate the \(\Delta H\), \(\Delta S\), and \(\Delta G\) of the following reaction at 1 bar, 298 K:

\[
\text{CaCO}_3^{\text{aragonite}} \rightleftharpoons \text{CaCO}_3^{\text{calcite}}
\]

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**Thermodynamic Data for the problem set**

<table>
<thead>
<tr>
<th>Phase</th>
<th>Component</th>
<th>(\Delta H^\circ) (kJ mol(^{-1}))</th>
<th>(S) (J K(^{-1}) mol(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphite</td>
<td>C</td>
<td>0.0</td>
<td>5.740</td>
</tr>
<tr>
<td>Diamond</td>
<td>C</td>
<td>1.85</td>
<td>2.37</td>
</tr>
<tr>
<td>Albite</td>
<td>NaAlSi(_3)O(_8)</td>
<td>-3921.02</td>
<td>210.04</td>
</tr>
<tr>
<td>Jadeite</td>
<td>NaSi(_2)O(_6)</td>
<td>-3011.94</td>
<td>133.47</td>
</tr>
<tr>
<td>(\alpha)-Quartz</td>
<td>SiO(_2)</td>
<td>-910.65</td>
<td>41.34</td>
</tr>
<tr>
<td>Olivine</td>
<td>Mg(_2)SiO(_4)</td>
<td>-2175.68</td>
<td>95.19</td>
</tr>
<tr>
<td>Orthopyroxene</td>
<td>MgSiO(_3)</td>
<td>-1546.77</td>
<td>67.86</td>
</tr>
<tr>
<td>Calcite</td>
<td>CaCO(_3)</td>
<td>-1207.30</td>
<td>92.68</td>
</tr>
<tr>
<td>Aragonite</td>
<td>CaCO(_3)</td>
<td>-1207.21</td>
<td>90.21</td>
</tr>
</tbody>
</table>

all values at 1 bar, 298 K