Assessment: Assignment 1
Due: 12 August 2013
Marks: 100
Value: 10 %

Introduction
Acetic acid is contained in a 100 mL aqueous solution with concentration $[CH_3CO_2H] = 0.5$ M (where 1 M = 1 mole/L). The (reversible) chemical reaction for acetic acid is:

$$CH_3CO_2H \rightleftharpoons CH_3CO_2^- + H^+ \tag{1}$$

and the equilibrium conditions are:

$$K_a = \frac{\left[CH_3CO_2^-\right]\left[H^+\right]}{\left[CH_3CO_2H\right]} \tag{2}$$

$$pK_a = -\log K_a$$

where $pK_a = 4.756$ for acetic acid in water. The pH

$$pH = -\log\left[H^+\right] \tag{3}$$

and concentrations of all species can be determined for the acetic acid solution from Eq. (2) by noting that *initially*:

$$\left[CH_3CO_2H\right] + \left[CH_3CO_2^-\right] = 0.5 \text{ M}$$

$$\left[H^+\right] = \left[CH_3CO_2^-\right]$$

The titrant sodium hydroxide (with concentration [NaOH] = 0.1 M) is slowly added to the acetic acid solution. Every mole of NaOH that is added produces one mole of Na^+ and one mole of OH^- and each mole of OH^- consumes one mole of H^+.

$$\text{This equation is blank for consistency with the original document} \tag{4}$$

The concentration of any species is given by (V is volume):

$$[X] = \frac{N_X}{V_{added} + V_{initial}} \tag{5}$$

The effect of H^+ being consumed by OH^- is that the equilibrium of Eq. (2) is disturbed and a new equilibrium must be formed. Let dC be the change in concentration caused by addition of dV litres of titrant, then the new concentrations that satisfy Eq. (2) can be obtained by solving for dC:

$$K_a = \frac{\left(\left[CH_3CO_2^-\right] + dC_{CH_3CO_2^-}\right)\left(\left[H^+\right] + dC_{H^+} - dC_{NaOH}\right)}{\left(\left[CH_3CO_2H\right] + dC_{CH_3CO_2H}\right)} \tag{6}$$

Note that Eq. (1) defines a relationship between the dC values:

$$-dC_{CH_3CO_2H} = dC_{CH_3CO_2^-} = dC_{H^+} \tag{7}$$

and because the reaction is forward, then dC_{H+} should be positive.

The equivalence point is where the number of moles of base is equal to the number of moles of acid. Above the equivalence point, a different chemical reaction occurs because all of the H^+ has been consumed:

$$CH_3CO_2{}^- + H_2O \rightleftharpoons CH_3CO_2H + OH^- \qquad (8)$$
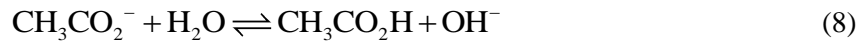
and the equilibrium conditions are ($K_b = K_w/K_a$ and $K_w = 1.0 \times 10^{-14}$ is the equilibrium constant for water):

$$K_b = \frac{\left[CH_3CO_2H\right]\left[OH^-\right]}{\left[CH_3CO_2{}^-\right]} \qquad (9)$$

Plot the pH of the acetic acid-sodium hydroxide mixture for the range of NaOH volumes over which the pH varies significantly. Note that the pH can be determined by (the equation using K_b is different because it nominally calculates pOH = 14 − pH):

$$pH = \begin{cases} pK_a + \log \dfrac{\left[CH_3CO_2{}^-\right]}{\left[CH_3CO_2H\right]} & \text{below equivalence point} \\[3ex] 14 - \left(pK_b + \log \dfrac{\left[CH_3CO_2H\right]}{\left[CH_3CO_2{}^-\right]} \right) & \text{above equivalence point} \end{cases} \qquad (10)$$

The midpoint is where half the volume of titrant required to completely neutralise the acid has been added (literally the number of moles of base is half the number of moles of acid): it is halfway to the equivalence point. Determine the midpoint using two methods; report the volume and pH of the midpoint and plot its location on the titration curve for both methods:
1. By taking half the volume of the equivalence point.
2. By locating when pH = pK_a.

By using two methods for determining the midpoint, you are **validating** the code (a global quality assurance control that the code overall produces the output you expect).

Requirements
For this assessment item, you must produce MATLAB code which:
1. Iterates through a range of volumes (incrementally add small volumes of NaOH).
2. Removes the appropriate number of moles of H^+ (if there is any left) or add the appropriate number of moles of OH^-.
3. Below the equivalence point, uses Eqs. (5)–(7) to determine the new concentrations of the species.
4. Above the equivalence point, uses Eq. (5) and the equivalent to Eqs. (6) and (7) appropriate for Eq. (9).
5. Calculates the pH.
6. Plots the pH versus volume of NaOH added.
7. Displays the volume and pH at which equivalence was reached and plots this point on the graph.
8. **Validates** the code by plotting the midpoint using both methods and displaying the volume and pH for both methods in the Command Window.
9. Saves an ASCII text file "titration.txt" with the first column being the volume and second column the pH.
10. Displays to the Command Window a brief discussion (fewer than 5 lines) stating the value you selected for the threshold level of [H^+] considered to be "completely consumed" and why you selected that value.
11. Has appropriate comments throughout.

Furthermore you must **verify** the code by using hand calculations to determine the pH after one incremental addition of NaOH and compare against your code's result. This is a local quality assurance control that the components of the code are operating within specifications. For ease of controlling significant figures, it is standard practice to use a larger increment than you would ordinarily specify in a computer code.

Hint
The results are very sensitive to the threshold level of [H^+] considered to be "completely consumed". You should experiment with different threshold values until you obtain results that are reasonable.

Submission
Submit your code and verification by the due date to the StudyDesk.

Note that:
- you should upload all of your files individually (not zipped together).
- you will NOT receive any confirmation of receipt. If you can see that the file(s) has uploaded, then you have successfully submitted your assignment. There is no need to click a "send for marking" button.

Assessment Criteria
Your code will be assessed using the following scheme.

Does the code run without error?	10 marks
Does the code have an appropriate header and comments?	10 marks
Plot appropriately presented? (e.g., axis labels, titles)	15 marks
Correct calculation of pH versus volume of NaOH and quality of code?	25 marks
Midpoint • Correct calculation using both methods? • Plot on figure? • Command window output? (e.g., descriptive, includes units)	15 marks
Text file output as required?	10 marks
Quality of discussion for selection of threshold level of [H^+]	5 marks
Quality of code verification using hand calculations	5 marks