EG3029 Chemical Thermodynamics

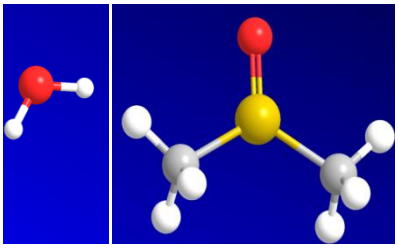
Lab Exercise II + III:

Excess Volume Determination

Problem:
Many substances do not exhibit ideal behaviour when they are mixed with each other. One prominent example is water in mixtures with other polar chemicals including methanol and ethanol. Such non-ideal effects result from strong intermolecular interactions and often manifest in significant deviations of the mixture properties from the ideal values. Needless to say, that knowing these deviations is of great importance for designing processes in many respects.

Fortunately, property deviations can be determined both numerically and experimentally in the form of excess properties. In the lab exercises we will determine excess volumes of water/dimethyl sulphoxide mixtures and compare calculated values with experimental ones.

The structures of the chemicals are illustrated in the figure and the material safety data sheets (MSDS) are available on MyAberdeen:



Lab exercise II:
Start UniSim and open a new case. Add water and dimethyl sulphoxide (DMSO) as components. Develop a strategy for determining the excess volume of binary water/DMSO mixtures. Using your approach determine the excess volumes of both systems with water mole fractions of 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1 with the following fluid packages:

- Lee-Kesler-Plocker
- Peng-Robinson
- Soave-Redlich-Kwong
- NRTL
- UNIQUAC

Using Excel, plot the difference V-V^{ideal} as a function of water mole fraction for all fluid packages.

Lab exercise III:

Preliminary note: Before this lab session you MUST read and understand the information given in the MSDS of the chemicals you are going to work with! In the beginning of the exercise you will be asked some questions about safety matters and you will not be allowed to carry out the experiments should you not be aware of potential dangers and hazards, as well as handling and disposal of the chemicals.

Using the analytical balances in the Chemical Engineering Teaching Lab prepare binary water/DMSO mixtures with water mole fractions of 0.1, 0.3, 0.5, 0.7, and 0.9. Make sure that the liquids have completely mixed. Determine the specific volume of all mixtures and the pure chemicals. In addition, calculate the ideal specific volumes.

Using Excel, plot the difference $V\text{-}V^{ideal}$ as a function of water mole fraction and compare the experimental results with the numerical ones from Lab exercise II. Which model does reproduce the experimental data best?

Deliverables:

Submission of worked example:
Write a report in the style of a short journal paper. It should contain (1) a cover page with your name, ID, the title of the lab, the course name etc., (2) a brief introduction, (3) a materials and methods section with an explanation of your approach to determine excess volumes with UniSim, and a description of the experimental method. (4) A results and discussion section with figures displaying data and findings should follow. (5) A final section should summarise the main results with concluding remarks. Prepare the report as PDF file and submit it through Turnitin. Submit your work 2 weeks after conducting Lab exercise III, at the latest. Penalties for late or non-submission are as follows: for late submission, 1 CAS mark will be deducted for each day late (including weekends); submission later than 7 days after the deadline will be considered as non-submission and a CAS mark of 0 will be awarded.

In addition, submit a paper copy of your report including a completed plagiarism cover sheet.

Note that the submitted work is part of the continuous assessment which will contribute 20% to your EG3029 mark.