3.020, Spring 2021
Thermodynamics of Materials
Problem Set 1

Massachusetts Institute of Technology
Department of Materials Science and Engineering

Due Friday, February 26, 2021 at 10am EST

We encourage you to work in groups. If you do so, please note the names of your groupmates on the first page of your solutions.

Remember to clearly present your solutions, including intermediate steps. We have provided a lot of space for each problem in this document, so please make use of it. Failure to show your work may result in reduced credit. Sloppy presentation may result in reduced credit.

1.1: Identifying Systems [9 pts]

Problem Statement: In this problem you will practice identifying systems, phases, and boundary conditions based on real-world situations. For each situation, please complete the following:

(i) Identify the best thermodynamic system that we could analyze to get the desired information. By "best" we mean the simplest, while still covering the essentials.
The system is the set of particles that you want to age to equilibrium. You should generally exclude the system's physical container from the system itself, instead using idealized boundary conditions (as in (ii)) to represent the container.

(ii) Characterize the system's boundaries as open or closed, rigid or non-rigid, and adiabatic or diathermal
Of course no actual system's physical boundaries are perfectly closed, rigid, or insulated, but these idealizations often simplify analysis, so we try to use them judiciously.

(iii) Identify the phases of interest in the system.
Recall that a phase is a thermodynamic system with uniform thermodynamic state throughout. Phases can be (and often are) made up of different species or constituents, but the arrangement and distribution of those species are uniform within a phase. Phase and composition are distinct (in fact, orthogonal) concepts that thermo neophytes often confuse. Here are some examples of phase names: solid solution of helium in uranium, mixture of water vapor and gaseous helium, pure solid gold, pure iron in a BCC crystal (α iron), liquid solution of silver in mercury.

(iv) Identify the components present in each phase

(v) Characterize each phase's boundaries as open or closed, rigid or non-rigid, and adiabatic or diathermal

1.1 continued...

(a) [3 pts] You're installing new flashing on a roof. You want to know whether it will oxidize.

(b) [3 pts] You're inside a car in winter. You want to know if your breath will condense on the window.

(c) [3 pts] You're making steel ninja swords. You want to figure out how much carbon you need to add to the molten metal in the crucible in order for secondary phase particles to precipitate when the cast metal cools.

1.2: Using Thermodynamic Data [10 pts]

Context: *When you encounter a thermo problem on-the-job someday, nobody is going to hand you the thermodynamic data and materials properties that you need to solve the problem. Not to worry, though; reliable data exists for many materials in massive databases. In the next two problems, and throughout the semester, we will intentionally leave out key properties to give you a chance to learn how to locate that data.*

Reputable sources include textbooks, the NIST Webbook/NIST-JANAF (https://webbook.nist.gov/chemistry/), the CRC Handbook of Chemistry and Physics (subscription, available through MIT Libraries), Springer Materials which includes the Landolt-Börnstein database (subscription, available through MIT libraries), and many more tabulated at:
https://libguides-mit-edu.libproxy.mit.edu/properties
Always cite the source of data that you use on problem sets, unless it is provided in the problem statement or in the textbook – we will look for citations when grading.

In this problem we use tools like heat capacity, thermal expansion coefficient, and compressibility. We often use these quantities in expressions like this:

$$Q = \int_{T_1}^{T_2} nC_P dT \tag{1}$$

In general C_p varies with temperature, making this integral nontrivial. Sometimes, one can approximate C_p as a constant with respect to temperature:

$$Q \approx nC_P(T_2 - T_1) \tag{2}$$

Problem Statement: You have a single crystal of magnesium oxide measuring $10 \times 10 \times 0.5$ mm^3 at STP (298 K and 1 atm).

(a) [2 pts] What is the mass of the sample, and how many moles of MgO does it have?

(b) [2 pts] What pressure is required to decrease the volume by 1% at constant temperature?

(c) [2 pts] What is the temperature-dependent heat capacity of MgO between 298 and 500 K? You can express your answer as a polynomial, or as a graph.

(d) [2 pts] Imagine heating the sample from 298 K to 500 K. How much heat is required, if the heat capacity were constant at the 298 K value?

(e) [2 pts] Now calculate the heat required using the actual, temperature-dependent heat capacity. By what percentage was your answer to part (d) wrong?

1.3: Conservation of Energy [11 pts]

Context: *Here's a chance to practice the First Law of Thermodynamics:*

$$\Delta U = Q + W \tag{3}$$

The ideal gas assumption below will allow you to use the ideal gas law and special approximations for the heat capacities. You may find DeHoff 4.2.4 useful.

Problem Statement: We are designing a type of cyclical engine that uses nitrogen as the working gas. The gas is initially at room temperature. We then heat it at a fixed volume of 1 m^3 so that its temperature rises to 500 K (step 1). The gas is then allowed to cool back to room temperature while maintaining a fixed pressure (step 2). The pressure is then relaxed back to its originally measured value of 0.2 MPa (step 3). The quantity of gas (*e.g.* the mole number) remains fixed throughout.

Note: This is not a Carnot engine

(a) [3 pts] Sketch the process on a (P,T) diagram, (P,V) diagram and a (T,V) diagram. Which of these graphs allows the easiest estimation of the mechanical work done during the cycle?

(b) [2 pts] Calculate Q, W and ΔU for step 1.

(c) [2 pts] Calculate Q, W and ΔU for step 2.

(d) [2 pts] Calculate Q, W and ΔU for step 3.

(e) [2 pts] As described above, this machine is a cooling device - it takes work as an input, and moves heat from colder regions to hotter regions, like your refrigerator. Now imagine running it in reverse, as a heat engine. What would be the efficiency of the engine? *Hint*: You don't need to do any new calculations of Q or W, your answers above can be used straightaway.