AE6050/Seitzman
Spring 2024
HW#2

Equilibrium Properties of Reacting Mixtures

- Homework solutions should be neat and logically presented, see format requirements (seitzman.gatech.edu/classes/ae6050/homeworkformat.html). Please note the requirement to draw some IMPLICATIONS/CONCLUSIONS from the results of each problem. This could be implications for a practical device, a comparison of the results of different parts of a problem, a physical interpretation for an equation, etc.
- To receive credit, show ALL work in the format described above. If you use equations from the notes, the class textbook or another book, please cite the reference.

1. **Specific Heat of a Reacting Gas**

   The specific heat of a gas mixture is most generally defined by $c_{p,mix} \equiv (\partial h_{mix}/\partial T)_p$. Based on the expression from class for the enthalpy of an ideal dissociating gas using the atom as the system zero:

   a) find an expression for the normalized specific heat, $c_{p,mix}/R_{A_2}$, of an ideal dissociating gas that includes only: α^*, T, θ_D (or their derivatives).

   b) simply your expression for part a) assuming $T << \theta_D$.

   c) sketch (a hand drawing is acceptable) how this normalized specific heat would vary with normalized temperature T/θ_D. Assume that pressure is fixed, and like the α^* curves shown in class, there is no dissociation below T/θ_D~0.04 and that dissociation is complete by T/θ_D~0.09. Your x-axis should be T/θ_D, and it should span the range 0.02-0.12. Include numbers on the y-axis which are estimates of the normalized specific heats at T/θ_D=0.03 and 0.10.

2. **Plasma Actuator - Saha Equilibrium Estimate**

   A colleague is working on a plasma actuator to replace flight control surfaces on a hypersonic vehicle. The actuator uses argon (Ar) gas. Her estimates suggest the actuator will only be effective if at least 4% of the Ar is ionized. The actuator is expected to operate at a pressure of 1.0 kPa.

   Use the following information for the ionization energies and electronic energy level data for Ar and Ar^+; do not use energy information from other sources.

	ε_{ioniz} (eV)*	$g_{o,el}$	$g_{1,el}$	$\varepsilon_{1,el}$ (eV)	$g_{2,el}$	$\varepsilon_{2,el}$ (eV)
Ar (Ar I)	15.760	1	8	11.580	4	11.778
Ar^+ (Ar II)	27.630	4	2	0.17754	2	13.479
Ar^{2+} (Ar III)	40.750	5	4	0.14878	5	1.7358

*An electron volt (eV) is the energy acquired by an electron accelerated through 1 Volt (=1.602×10^{-19} J) – but it can be converted to temperature units by dividing by Boltzmann's constant (i.e., ε/k). Thus 1 eV ≈ 11,604.5 K.

a) Assuming equilibrium and no doubly ionized Ar is present, what is the minimum required operating temperature (i.e., of the gas)?

b) What would be the electron number density at these conditions?

c) We want to check our assumption that doubly ionized Ar (Ar^{2+}) can be neglected. To do this, estimate the ratio of the number densities of the Ar ions, i.e., $n_{Ar^{2+}}/n_{Ar^{+}}$ assuming our original assumption was correct and that the values obtained from steps a) and b) are accurate.

d) What temperature would be required to produce the same 4% ionization level if the pressure was increased to 1.0 bar? Use the same assumptions as in a).

In the following problems, you will be calculating properties of gas mixtures of CO_2, O_2, CO and O with an O:C ratio of 5. You will need to develop your own computer tool/program to develop the ability to perform the calculations; do not use any existing chemical equilibrium software. Any general programming or equation solving tool you use is acceptable, ***BUT*** *be aware that whatever you use, you will be using it again in future assignments to solve reacting flow problems (so make it general enough to help you later).*

The molecular properties of CO_2, O_2, CO and O are given in the table below; you can assume each is a thermally perfect gas. **For the following problems, do not use data from any other source.**

	MW	θ_r (K)	$\theta_{vib,1}$ (K)	$\theta_{vib,2}$ (K)	$\theta_{vib,3}$ (K)	$g_{0,el}$	$g_{1,el}$	$\theta_{1,el}$ (K)	$g_{2,el}$	$\theta_{2,el}$ (K)	$g_{3,el}$	$\theta_{3,el}$ (K)	$\Delta h_f(0K)$ (kJ/mol)[a]
CO_2	44.01	0.560	1915	960.6[b]	3381.	1	3	88,194-	---	----	---	----	-393.151
CO	28.01	2.80	3120	---	---	1	2	93,507	---	----	---	----	-113.805
O_2	32.00	2.08	2270	---	---	3	2	11,393	1	18,985	1	47,563	0
O	16.00	---	---	---	---	5	3	228	1	326	5	22,831	246.790

[a] The formation enthalpy is the amount of energy required to form a mole of a species from its "elements." The formation enthalpies (at 0 K) given here are from the JANNAF tables, which use O_2 and C(s) as the elemental forms of oxygen and carbon (i.e., it assumes that O_2 and C have zero chemical energy). Also mol here means gmol (not kmol).

[b] This is a doubly degenerate bending mode, i.e., there are two vibrational (bending) modes have the same characteristic frequency.

3. Equilibrium Composition

Calculate and plot the (equilibrium) composition in mole fractions of our gas mixture at 0.10 atm as a function of temperature from at least 300 to 6000 K <u>using partition function based equations</u>, e.g., to determine K_p values.

4. **Mixture Enthalpy**

   Calculate and plot the (equilibrium) enthalpy (per unit mass) of this gas mixture (at the same pressure of 0.10 atm) as a function of temperature from at least 300 to 6000 K, using expressions based on statistical mechanic models.

5. **Mixture Entropy**

   Calculate and plot the (equilibrium) **absolute** entropy of this gas (again at 0.10 atm) as a function of temperature from at least 300 to 6000 K using partition function based equations. Plot both the entropy (per unit mass) and the normalized entropy s/R.

Extra Credit

Calculate and plot the (equilibrium) specific heat (c_p) of this gas and the normalized specific heat (c_p/R) as a function of temperature from at least 300 to 6000 K. Use an (accurate) numerical difference approach to calculate c_p based on your enthalpy results. On your graph(s), also show c_p/R assuming all energy modes of the gas are frozen except translation and rotation, based on the composition of the gas at 300 K.