

ME EN 5830/6830: Aerospace Propulsion
Problem Set #2: Combustion I and II
Due date: 01/23/2024 by 11:59pm

Submission

Assignments can only be submitted on Gradescope, which can be accessed through Canvas. If you have any questions about submission, please email the class TA, John Gardner at u0763966@utah.edu. Submissions will be automatically locked at the due date given above.

Introduction

This problem set primarily covers the material from Lectures 3 and 4. The goal is for students to work with mixtures of ideal gases and chemical reactions. Upon completion of the assignment, students should be able to:

- Determine state variables in a thermodynamic process for a mixture of ideal gases
- Compute the adiabatic flame temperature for a constant pressure system by hand
- Use software to compute combustion properties

The (adiabatic, constant pressure) first law with chemical reactions

Recall that when we derived the first law for an adiabatic, constant pressure system, we said:

$$dh = 0$$

We can take this as a fact. However, in problem set #1, because the JANAF table provided values per mole rather than per mass, you may have also assumed that:

$$d\bar{h} = 0$$

While the above equation is true for an inert mixture, it is invalid for reacting mixtures. Proof:

$$\bar{h} = h\bar{m} = hM/N$$

Then,

$$d\bar{h} = d\left(\frac{hM}{N}\right)$$

Applying the chain rule,

$$d\bar{h} = \frac{M}{N}dh + \frac{h}{N}dM + hMd\left(\frac{1}{N}\right)$$

We know that for this process $dh = 0$, and given conservation of mass, that $dM = 0$. Then,

$$d\bar{h} = hMd\left(\frac{1}{N}\right)$$

Since the number of moles of reactants does not necessarily equal the number of moles of products, the right-hand side of the above equation is not necessarily zero. Therefore, we cannot assume that $d\bar{h} = 0$ when considering chemical reactions. Be very careful about converting units. The safest thing to do is to immediately convert each quantity from the JANAF tables to be per mass before using them in equations.

Computing Adiabatic Flame Temperature

For an open system with no heat *crossing system boundaries*, we can simplify the first law to

$$dh = 0$$

Then for our combustion reactions, this further simplifies to

$$h_{\text{reac}}(T_{\text{reac}}) = h_{\text{prod}}(T_{\text{prod}})$$

For a general number of reactants (R1, R2, ...) and products (P1, P2, ...), we can expand the above equation out to

$$Y_{R1}h_{R1}(T_{\text{reac}}) + Y_{R2}h_{R2}(T_{\text{reac}}) + \dots = Y_{P1}h_{P1}(T_{\text{prod}}) + Y_{P2}h_{P2}(T_{\text{prod}}) + \dots$$

In the above equations, Y_{R1} is the mass fraction of reactant species 1 in the reactants, and h_{R1} is the enthalpy of species 1 in the reactants. We can expand any of these enthalpy terms into two parts, a sensible enthalpy and an enthalpy of formation. For example:

$$h_{R1}(T_{\text{reac}}) = \Delta h_{s,R1}(T_{\text{reac}}) + h_{f,R1}(T_{\text{ref}})$$

$$h_{P1}(T_{\text{prod}}) = \Delta h_{s,P1}(T_{\text{prod}}) + h_{f,P1}(T_{\text{ref}})$$

Note that in the above equation, the sensible enthalpy (energy stored in molecular kinetic energy) is evaluated at the gas temperature, whereas the enthalpy of formation (energy stored in molecular bonds) is evaluated at the reference temperature. Below is a screenshot of a JANAF table for an arbitrary molecule

T/K	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.	0.	INFINITE	-10.024	-66.911	-66.911	INFINITE
100	33.258	149.500	216.485	-6.698	-69.644	-64.353	33.615
200	33.473	172.577	189.418	-3.368	-72.027	-58.161	15.190
250	34.216	180.113	186.829	-1.679	-73.426	-54.536	11.395
298.15	35.639	186.251	186.251	0.	-74.873	-50.768	8.894
300	35.708	186.472	186.252	0.066	-74.929	-50.618	8.813
350	37.874	192.131	186.694	1.903	-76.461	-46.445	6.932
400	40.500	197.356	187.704	3.861	-77.969	-42.054	5.492
450	43.374	202.291	189.053	5.957	-79.422	-37.476	4.350
500	46.342	207.014	190.614	8.200	-80.802	-32.741	3.420

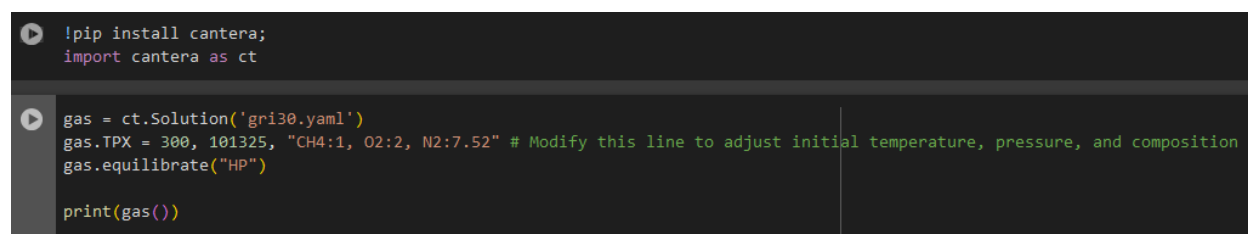
Let's say, hypothetically, this JANAF table corresponded to molecule R1, and that $T_{reac} = 500$ K. Then, the sensible enthalpy (in molar form) would be given in the fifth column and would be $\Delta \bar{h}_{s,R1}(T_{reac}) = 8.200 \frac{kJ}{mol}$. The (molar) enthalpy of formation, evaluated at the reference temperature $T_{ref} = 298.15$ K would be given by the sixth column of the JANAF table and would be $\bar{h}_{f,R1}(T_{ref}) = -74.873 \frac{kJ}{mol}$.

If you look again at the governing equation for this system, you will notice that on the reactants side of the equation, all terms are either a function of T_{reac} , or T_{ref} . These are both known quantities, and therefore you can explicitly evaluate the LHS. The RHS, however, is a function of T_{prod} and T_{ref} . While we know the reference temperature, T_{prod} is the adiabatic flame temperature and is the quantity we wish to solve for. Therefore, we make an initial guess for T_{prod} , evaluate the RHS, and see how close we are to the LHS. We then pick another temperature, re-evaluate the RHS, and see whether the RHS is becoming closer to the LHS. Continue this iterative process to find which two values of temperature give you a RHS that bounds the LHS, and then linearly interpolate for the temperature that gives you LHS=RHS. This is your adiabatic flame temperature.

Using the online Cantera calculator

Cantera (cantera.org) is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Rather than installing a local copy, we will use google colab (an online hosted Jupyter notebook) to run the software online and compute adiabatic flame temperatures. I have pre-written a Python script for you that can be accessed at the following link: <https://colab.research.google.com/drive/1OHP3w4dvTYWpCuyMdzSfG8vYtMLdyL2-?usp=sharing>. Using the script for this assignment involves the following steps:

1) Click the link above to open google colab. You should see something like below. Feel free to save your own copy of the script as you play around with it. You should not be able to modify and save the original.



```
!pip install cantera;
import cantera as ct

gas = ct.Solution('gri30.yaml')
gas.TPX = 300, 101325, "CH4:1, O2:2, N2:7.52" # Modify this line to adjust initial temperature, pressure, and composition
gas.equilibrate("HP")

print(gas())
```

2) Press the first play button (top left) to run the first block of code – this will install the required Cantera libraries in google colab.

3) Set the desired initial state on the line starting with “gas.TPX”. After the equals sign, the first number is the initial temperature (Kelvin), followed by an initial pressure (in Pa), and then an initial composition. Note that you can modify, add, or remove molecules to and from the list. For each molecule, the number after the colon represents the number of moles of that molecule (e.g., CH4:1, O2:2 means a mixture of 1 mole of CH4 and 2 moles of O2).

4) Press the second play button to run the second block of code. The output will give you the final state after reaching chemical equilibrium, including variables like the temperature and composition of the gas.

Assignment

Problem #1: Consider a mixture of ethylene (C_2H_4) and air with an equivalence ratio of 1.2.

- a) Based on the simplest approach for rich combustion discussed in Lecture 4 (approach #1), what do you expect the combustion products of this mixture to be? Why?
- b) Write out and balance the governing reaction for this mixture and equivalence ratio assuming the products from part a).

- c) Compute the mole fractions and mass fractions of each chemical species for the reactants and products. Report them in a table like the following, where the relevant chemical species names are added to the left column:

	X	Y
R1:		
R2:		
R3:		
P1:		
P2:		
P3:		
P4:		

- d) Assume that the reactants are originally at $T_0 = 800$ K and $p_0 = 10$ atm and that combustion occurs at constant pressure. For this problem, you may assume that specific heats are constant. Assume the value of specific heat for each chemical species has a value equal to $c_{p,i}(T_{ref})$ taken from the JANAF table (e.g., $c_{p,O_2} = 29.376$ J/mol-K). Compute the adiabatic flame temperature. Recall $\Delta h_{s,i}(T) = c_{p,i}(T - T_{ref})$.
- e) For the same initial conditions, recompute the adiabatic flame temperature assuming specific heats are **not** constant. Recall from Lecture 3 that this is an iterative process. Please use a program like Excel or MATLAB and include a screenshot of your worksheet or code. You should start guessing at a temperature of 2500 K.
- f) **Conceptual:** Assume that the reactants instead start at $T_0 = 800$ K and $p_0 = 20$ atm. What is the adiabatic flame temperature if specific heats are not constant? Why?
- g) **Conceptual:** If combustion in this system occurred between fuel and pure oxygen rather than fuel and air (i.e., the nitrogen molecules were simply removed from both sides of the equation), how would the adiabatic flame temperature change? Why? Recall that we assume N_2 doesn't react.
- h) Using Cantera, compute the final temperature and composition at equilibrium at the same conditions as e). How do the temperature and composition compare to your answers from Problem 1? Are any additional species present in sufficient quantities to be worth considering?
- i) Repeat step h), but with the elevated pressure given in step f). How does the final temperature compare to h)? Explain why this is conceptually different than what you (hopefully) found in part f). If you are struggling, think about the differences in rich combustion approach #1 vs. #2 and #3 from lecture 4.