ME 370B
Energy Systems II:
Modeling and Advanced Concepts

C.F. Edwards
Winter 2023

Project #2: Chemical Exergy and Exergy Analysis Functions

Individual assignment, due as a PDF file via Canvas, Thursday, January 26, 11 PM

Exergy is the work potential of a resource. The ability to calculate and subsequently manipulate resource exergy is a key component of understanding advanced energy systems. In this assignment you will explore how to calculate chemical exergy and the effect that choices about the environmental state can have on the value of an energy resource. We will accomplish this by building a couple of Matlab functions to evaluate the exergy of arbitrary fluid streams. We will also build functions that return the heating values (lower and higher) of an arbitrary gas stream. These functions (and the device models from last week) will be used in next week's assignment to analyze a natural gas, combined-cycle, power plant.

The Objectives

(1) to gain experience calculating chemical exergy,

(2) to understand the effects of choices about the dead state,

(3) to build exergy-analysis tools that can be applied to general systems, and

(4) to begin to develop understanding of exergy management of resources.

The Assignment

Individual code and write-ups are required for this assignment. You are encouraged to work with your group to develop understanding and methodology, but you must write your own code.

(1) 25 Points Write a function that returns the lower heating values of a Cantera GRI30 ideal gas object *of any composition*. Use 25°C, 1 atm as the reference state and assume the heating value is determined by a flow calorimeter (not a constant-volume calorimeter). In keeping with Cantera styling & conventions, name your function *LHV_mass*.

Make a copy of your function and modify it so that it returns the higher heating value. Name this function *HHV_mass.*

(2) 25 Points Write a function *exergy_mass* that returns the mass-specific internal exergy of a GRI30 ideal gas *of any composition* and *at any state*.

Make a copy of your function and modify it so that it returns the mass-specific flow exergy. Name this function *flowExergy_mass.*

Use your functions to generate a table of exergy and heating values for the fluids list below. In each case list the fluid name and the four values generated by your functions (LHV, HHV, mass-specific internal exergy, mass-specific flow exergy).

```
Hydrogen                        T = 25°C, P = 101325 Pa
Carbon Monoxide                 T = 25°C, P = 101325 Pa
Methane                         T = 25°C, P = 101325 Pa
Propane                         T = 25°C, P = 101325 Pa
Nitrogen                        T = 25°C, P = 101325 Pa
Oxygen                          T = 25°C, P = 101325 Pa
Carbon Dioxide                  T = 25°C, P = 101325 Pa
Natural Gas                     T = 25°C, P = 101325 Pa
                                Composition from Project 1
A Simplified Syngas             T = 25°C, P = 10 MPa
                                x(CO) = 0.4, x(H2) = 0.6
Engineering Air                 T = 25°C, P = 101325 Pa
                                x(O2) = 0.21, x(N2) = 0.79
Compressed Engineering Air      T = 25°C, P = 10 MPa
Cold Engineering Air            T =  0°C, P = 101325 Pa
Warm Engineering Air            T =650°C, P = 101325 Pa
```

Using the following fluid (environmental air) as the dead state:

```
Temperature:  25°C         Pressure:   101325 Pa
Composition:  Species:     Mole Fraction:
              N2           0.757223
              O2           0.202157
              H2O          0.031208
              Ar           0.009015
              CO2          0.000397
```

(3) 25 Points Plot the effect of dead-state relative humidity on the chemical exergy of carbon monoxide, methane, and hydrogen. Plot your results as the ratio of the exergy at the dead state at any given *RH* to the exergy with the dead state saturated (*RH* = 100%) vs. *RH*. Use the same dead state *T* and *P*, and the same $N_2/O_2/Ar/CO_2$ proportions as listed in Part 2. Plot your results over a range of relative humidity from 0.01% to 100%.

(4) 25 Points Write functions that return the mass-specific internal exergy and mass-specific flow exergy of a real fluid object (e.g., water, R134a, or CO_2) in Cantera.

Write a script that plots an exergy-entropy diagram (*x*-*s*) for water (internal exergy, not flow). Use the same contours as the *T*-*s* and *u*-*s* diagrams given in the sample file on Canvas so that you can make a direct comparison. Consider how these three diagrams relate to each other. Why does each look the way it does? (No written response required. I just want you thinking about this.) Please include a description of your dead state for water and a brief explanation (just a paragraph) as to why you made this particular choice.

Once you are finished with the plot, merge these scripts with your *exergy_mass* and *flowExergy_mass* functions from above so that you have general functions that can deal with any GRI30 gas, or water or CO_2 as pure substances.

The Write-Up

Only the plots/table and brief answer (on Part 4) are required. Also please include a statement of how much time was spent on each part and your opinion of the most and least useful aspects of the assignment.

The Deliverables

(1&2) A table with exergies and heating values

(3) A plot of exergy vs. dead state relative humidity for three fuels

(4) *T-s* and *u-s* diagrams for water (from Canvas scripts)
x-s diagram for water
Definition of dead state with explanation

Some Cantera Hints

Cantera and Matlab sometimes (but not always) have a problem solving the heating value problem at 25°C. The symptom is that Matlab crashes. If this happens, change the temperature to 300 K. This makes no difference in terms of the heating value but seems to avoid whatever the condition is that causes the crash.

In using the commands *speciesIndex* and *elementIndex* with argon, Cantera uses the string “AR” for argon as a molecular species and “Ar” for argon as an element. While the difference due to miss-assigning argon is not usually large (the argon in the dead state has a small effect on chemical potentials), this can account for disagreements between codes on exergy values.