ChE 641
Helpful Hints on the Equilibrium Programs

A. Available Codes (recommended codes are in bold)

- **NASA-CEA (see class website)**
- **EDWRDS**
  - (available on VAX and UNIX; groups/che641/equil/edwrds)
  - **PC version available (see class website)**
- **GasEq (**http://www.c.morley.dsl.pipex.com/**)**
- **Cantera (**see Dr. Lignell**)**
- NASA-Lewis
  - UNIX version (groups/che641/equil/nasalewis)
  - METC version (groups/che641/equil/metcec)
  - SuperBurn (very user friendly; see Dr. Scott Hill)
- PEP (Navy version acquired by Dr. Beckstead)
- Super-Burn (Developed by Scott Hill)

B. Getting equilibrium codes to read the molar quantities from the reactant "cards"

NASA-Lewis (UNIX) and NASA-Lewis (METC)

> "As an alternative, all reactants may be designated as fuel or oxidant. In this case, the relative amounts of the reactants are completely specified by the values on the REACTANT cards." (from "METCEC - User's Manual," P. A. Nicoletti (1986).

This means that all of the feed species must indicate "F" uniformly or "O" uniformly in order for the program to use the molar ratios in the input file. These two programs do not read the reactant cards if a mixture of "F" and "O" specifiers are used.

C. Units

NASA-Lewis (METC)

Units here are cal/gmol. The units in the other NASA-Lewis files are kJ/kgmol.

Super-Burn

The units on the enthalpy of formation say kJ/kg, but really mean kJ/kgmol.

D. Input Command Files

UNIX programs

UNIX programs that read from the screen can easily be used in a mode that reads from a file. The same goes for printing the screen information to a data file. If *inp* is the name

of the input file, and *out* is the output file, and I was running the program *edconv* in UNIX, I could type the following:

edconv < inp > out

This would run the *edconv* program, and the program would read the information from the file named *inp* and write any screen information to the file *out* instead of the screen. This works in UNIX on any type of program! (I used italics, but you do not use italics on the computer).

E. Translations of programs

EDWARDS/UNIX

The version of EDWARDS on the UNIX machines has been modified and now should give the same answers as the NASA-Lewis program.

F. Manuals

NASA-Lewis/METC (metcec)

I obtained a copy of the user's manual for the METC NASA-Lewis code. You may borrow this manual for photocopying purposes, or else write to DOE. The code uses a namelist at the end of the *ftn01* file in my /equi/metcec directory. The JANAF data are in *ftn30* . The relevant namelist commands are attached on the next page. Remember that comments **A**, **B, and C** above are pertinent. A sample namelist input command follows:

```
NAMELISTS
  $INPUT  P=4.5 , ERATIO=T , MIX=1.087 , TP=T , TRACE=1.E-7 ,
          T=2817.,2400.,2000.,1800.
  $END
```

Six sample problems are in my /equil/metcec subdirectory, named *prob1.dat*, etc.

The metcec program uses a Makefile to compile the different subroutines, if you are getting a copy for yourself.