Appendix B
Tutorial

This section is intended to give a brief introduction to navigating through VTEC and becoming familiar with the interface. User entries in VTEC are denoted by a

VTEC prior to the instruction. Some figures in this section may have undergone slight revisions since this writing.

To start VTEC,

VTEC Type **VTEC** from the DOS prompt

VTEC will run faster if it is executed outside of a windows environment. The program will load and check for the needed supporting font files, thermochemical database and other supporting files. The introductory screen will appear.

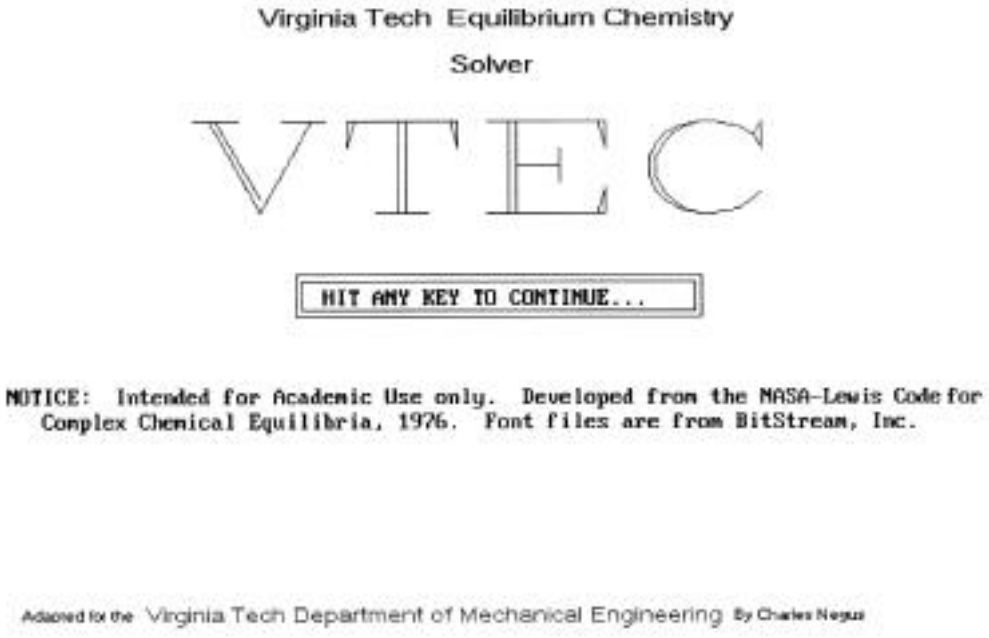

FIGURE B.1 VTEC Introductory screen

VTEC Press any key to continue. When asked if you wish to load a file or manually enter data, type **M**.

The VTEC input page will come up showing empty Reactants, Problem, Omit / Only, and Options boxes. These may be specified in any order, but it usually makes sense to start with the reactants.

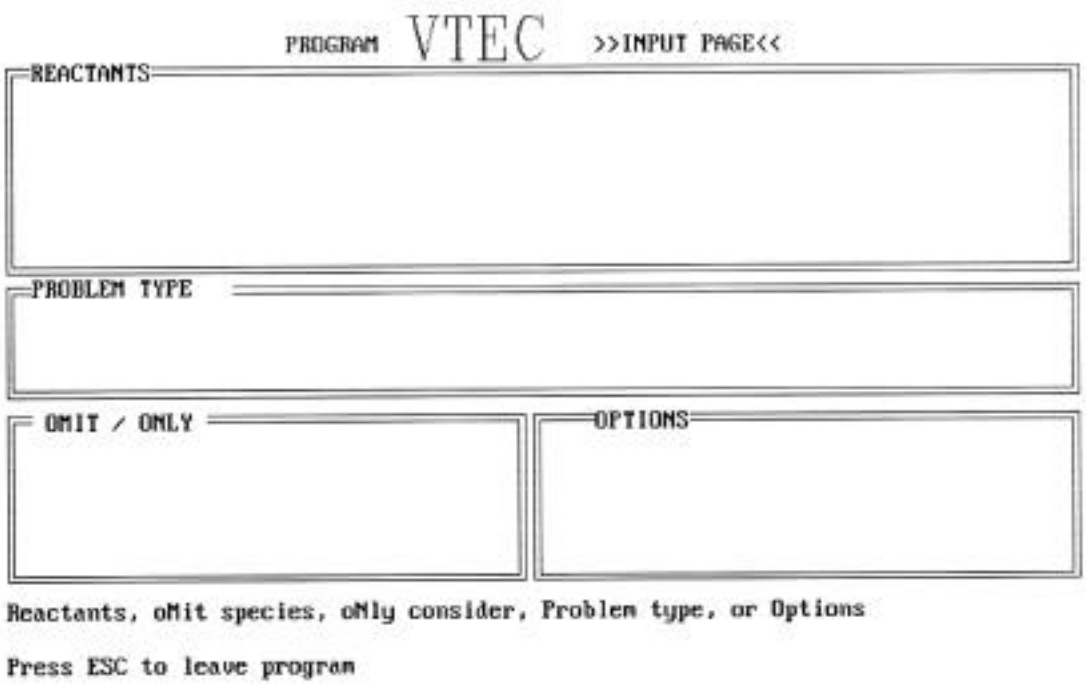

FIGURE B.2 Input Page

VTEC Type **R** to specify the reactants card. A prompt will appear asking for the number of reactants you wish to enter. Enter **2**. The program now asks to choose between specifying reactants in terms of weight or molar quantities. Enter **2** for moles.

The first reactant can be entered now. When entering the reactant, each element in each species requires an atomic coefficient. Water is H2O1, not just H2O. As we will see, this is not true when specifying the Omit or Only data.

VTEC Enter **C8H18**. When asked for the number of moles of species, enter **1**. Since liquid octane at standard temperature is in the thermochemical database, it is not necessary to enter the enthalpy of this reactant. Type **N**.

If the reactant temperature was outside the range of temperatures found in the database, the reactant enthalpy could not be calculated by the program and would have to be entered.

VTEC Enter **L** for the phase of the reactant. The octane will enter the combustion chamber at a standard temperature of 25°C or 298K. Enter **298.15**.

The first reactant has now been entered into VTEC.

VTEC Enter **O2** for the second reactant. Enter **12.5** for the number of moles of oxygen. This is the stoichiometric amount for complete combustion into CO_2 and H_2O. The enthalpy of oxygen does not need to be entered: type **N**. To designate the oxidant as a gas, type **G**, then enter **298.15** to indicate oxygen is also at standard temperature.

The reactants have now been entered. We will next define the problem as a combustion, or constant enthalpy (HP) problem.

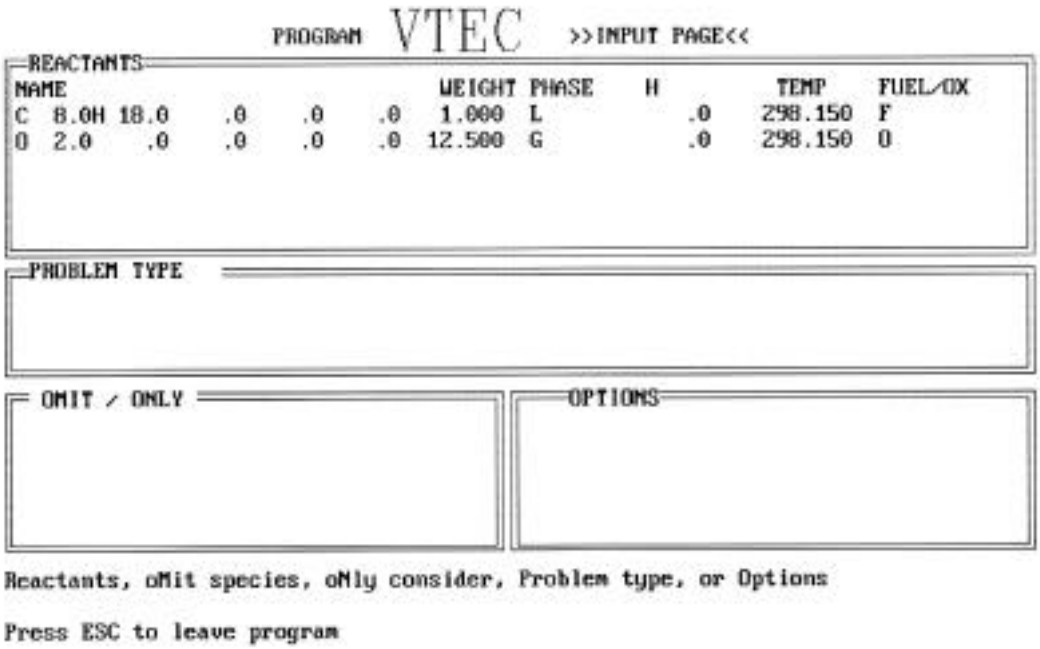

FIGURE B.3 Reactants information

VTEC Type **P** to specify the problem type.

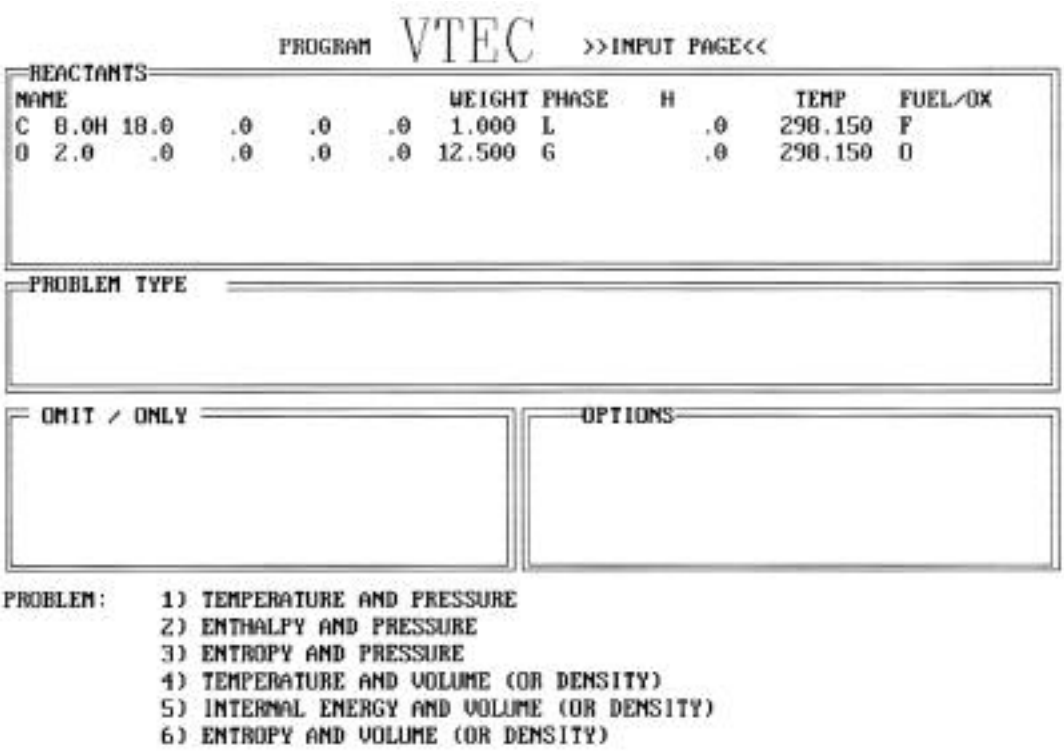

FIGURE B.4 Problem Type

VTEC Type **2** to pick “Enthalpy and Pressure (HP)” from list. Type **2** to run two pressure cases. Enter **1** when asked for the first pressure. Enter **10** when asked for the second pressure.

The middle box should now be labeled “Problem Type HP”. VTEC can now calculate the equilibrium compositions for this problem.

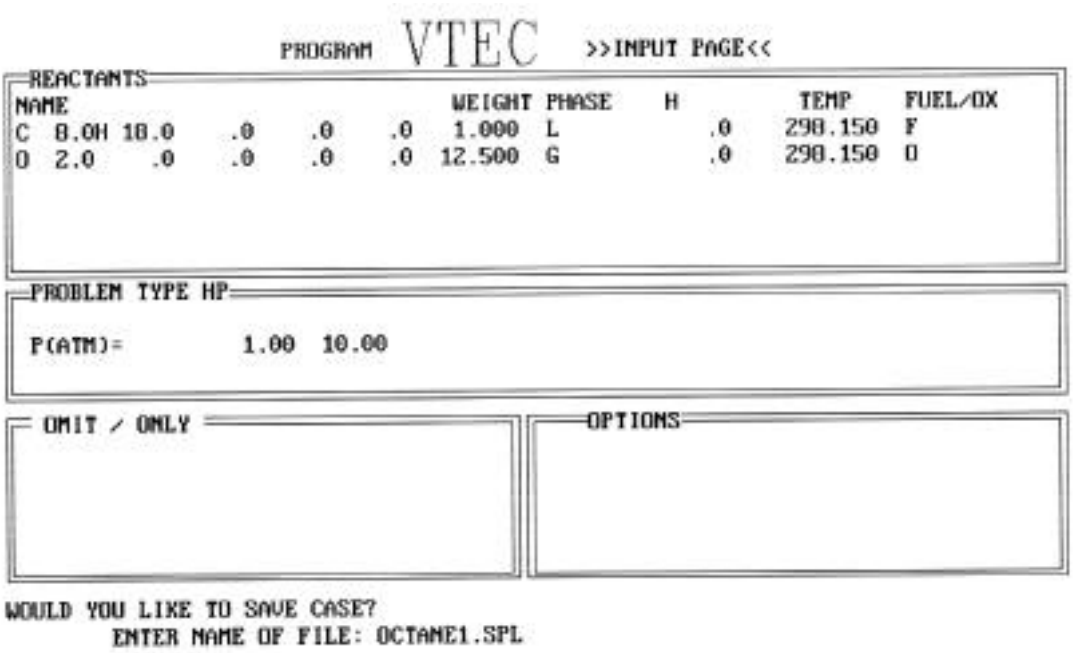

FIGURE B.5 Completed Input

VTEC Type **D** to indicate the problem is ready to run. When asked to save case, type **Y**. Enter **OCTANE1.SPL**.

After the input has been saved as a text file, the output page will appear listing the equilibrium products and their compositions for combustion at 1 and 10 atmospheres. An output file called "OCTANE1.OUT" is also created that contains the equilibrium information displayed on the screen as well as some thermodynamic properties of the products. Other species that were considered but whose mole fractions were less than 0.000005 are listed in the lower box, but are not written to the output file. The highlighted arrows on this box indicate that there are more species that can be scrolled through using the arrow keys.

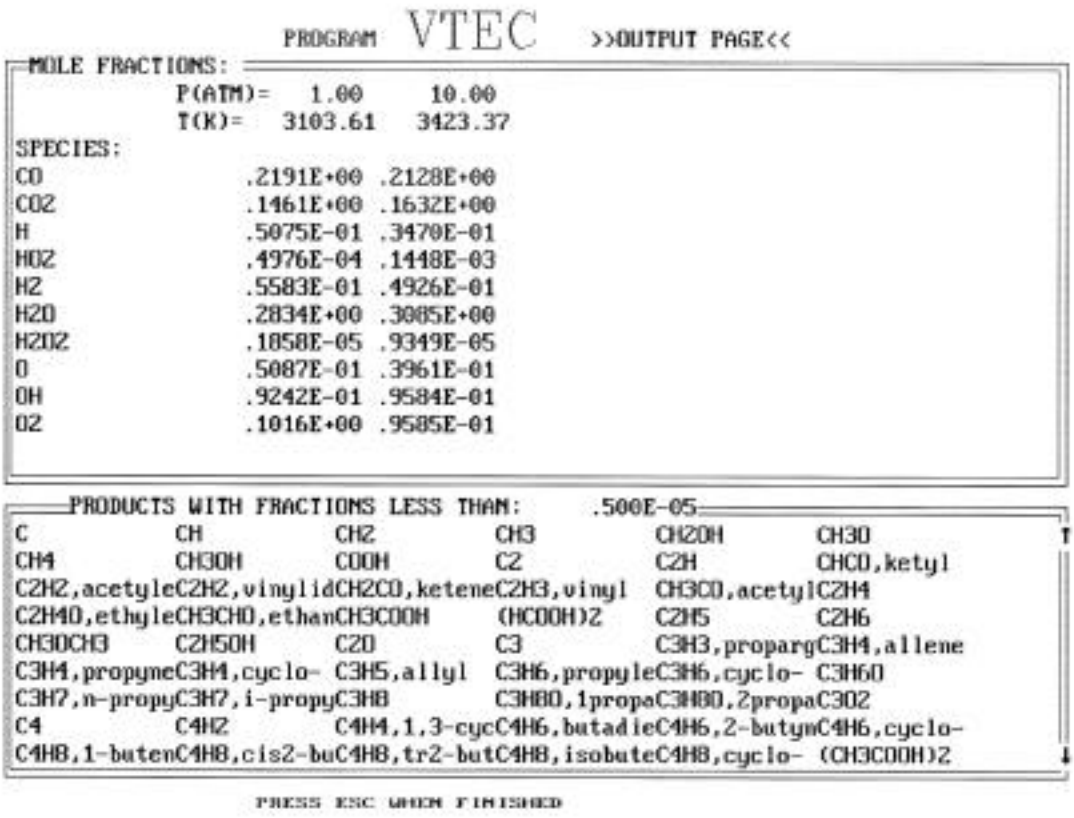

FIGURE B.6 Output

VTEC When you have viewed the products, press the **ESC** key. Type **R** to indicate you would like to run another case. Type **Y** to indicate you would like to re-run the last case.

The input screen reappears with the previous problem loaded. For this case we will simulate the results of an equilibrium constant approximation using seven possible products: CO_2, CO, H_2O, H_2, OH, O_2, and C_8H_{18}. Octane and oxygen will be considered because VTEC usually requires that the reactants be among the species considered in the system. We will run this case for four different equivalence ratios.

VTEC Type **N** to specify the only species that you would like considered. When asked for the number of species to be considered, enter **7**. Enter each of the following species:

C8H18(L),n-octa

O2

CO2

CO

H2O

H2

OH

These species now appear in the box titled “ONLY”.

VTEC Type **O** to enter the options menu. Type **E** to select equivalence ratios. Enter **3** when asked for the number of mixture ratios. Enter the ratios: **0.75, 1.0, 1.25**.

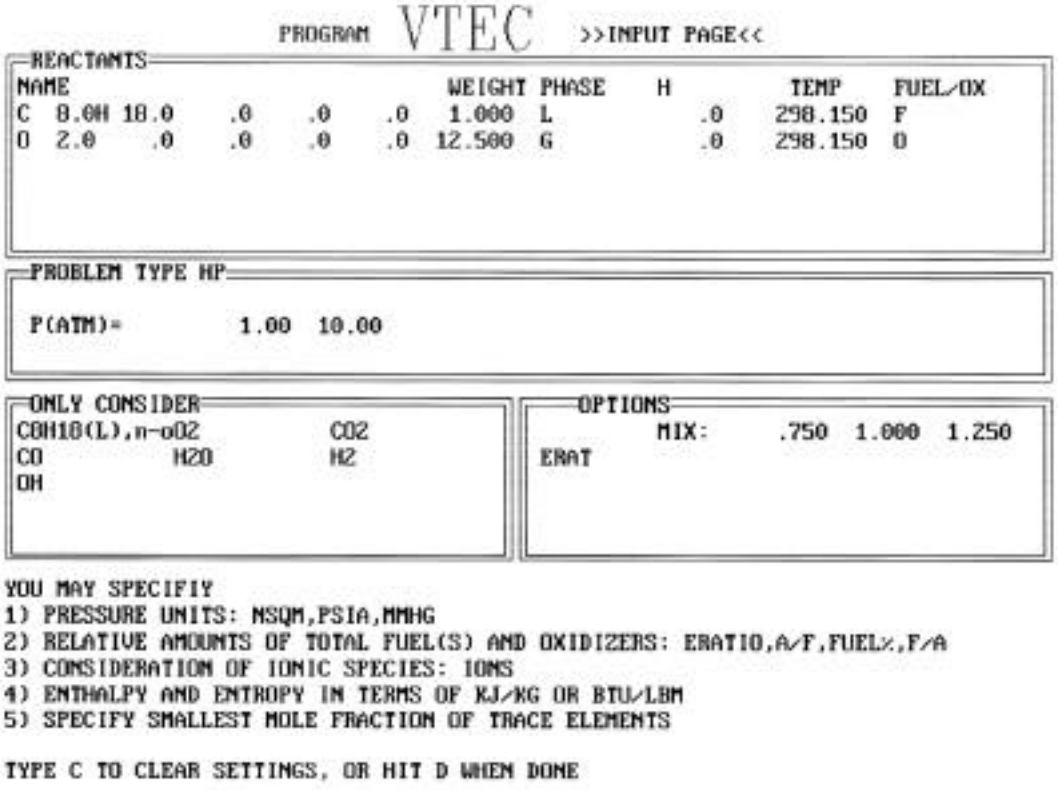

FIGURE B.7 Problem constrained by **ONLY** for three values of **ERATIO**

VTEC will calculate the necessary molar quantities of the fuels and oxidants to achieve each of the three ratios above. Octane was marked with an **F** to distinguish it as a fuel while oxygen was marked **O**. The mole quantities necessary for each equivalence ratio will override those entered in the reactants box.

VTEC Type **D** to close the options box. Type **D** again to run the case.

If this case is not saved, the input and output will be saved in the files “LAST.RUN” and “LAST.OUT”, respectively. The output screen reappears with new mole quantities. The first equivalence ratio is displayed in the top right corner.

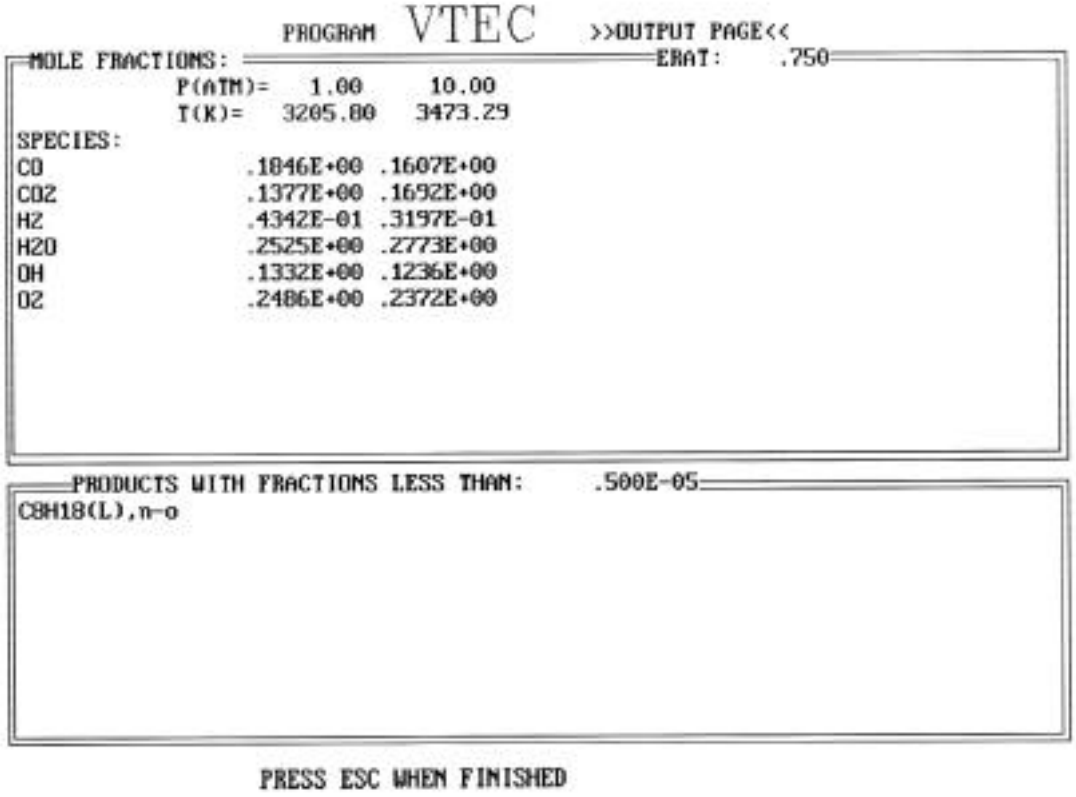

FIGURE B.8 Output with constrained products

VTEC Press the **ESC** key to see the equilibrium results using the other equivalence ratios. Press **ESC** to exit the program.

The *.OUT files generated from these problems (OCTANE1.OUT and LAST.OUT) can be printed to keep a record of these results