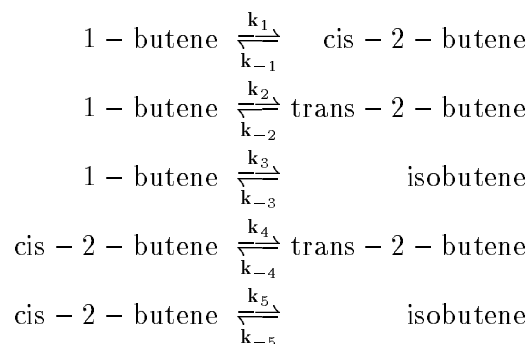


The first problem will illustrate row and column vector entries, simple matrix calculations, and a screen prompt for input. The second problem illustrates variable types, function calls, functions (subroutines), solution of an ODE, and plotting functions.

### Problem 1

Butene isomerization reactions are shown below.



The thermodynamic data are

Components	$\Delta G_f^{298K}$ (kcal/mole)	$\Delta H_f^{298K}$ (kcal/mole)	A	B ( $\times 10^2$ )	C ( $\times 10^5$ )	D ( $\times 10^9$ )
1-butene	17.04	-0.03	-0.7156	8.442	-4.756	10.67
cis-2-butene	15.74	-1.67	0.1051	7.058	-2.433	-0.1472
trans-2-butene	15.05	-2.67	4.379	6.128	-1.676	-2.148
isobutene	13.88	-4.04	3.865	6.702	-2.608	2.174

where the component heat capacities in cal/gmole-K can be calculated using

$$C_{pj} = A_j + B_j T + C_j T^2 + D_j T^3$$

Generate an M-file that will compute the component heat capacities and the component heats of formation.

### Problem 2

The thermal cracking of propane



is first order in the concentration of  $\text{C}_3\text{H}_8$ . The reaction will be conducted in an isothermal PFR operating at  $800^\circ\text{C}$  and at a constant pressure of 1 atm. At  $800^\circ\text{C}$  the rate constant is  $4.1 \text{ sec}^{-1}$ . The feed contains a steam diluent (3 moles of steam

fed per mole of propane fed). You need to find the reactor volume to produce 300 million pounds of ethylene per year that operates at a propane conversion of 95%. This design condition results in a propane feed rate ( $N_{p,f}$ ) of 0.358 lb-moles/sec. (The answer is 1,730 ft<sup>3</sup> so we can use this to set the print interval in the program. In general you would not know this and would have to change the range over which you integrate the equations until you arrived at an answer.) To determine the concentration (or molar flowrate) of each component you need to solve the appropriate design equation, which for a PFR is

$$\frac{dN_j}{dV} = R_j$$

This equation is written for each component and the set of ODEs is solved subject to the initial conditions. The rate of production of each component is

$$R_j = \sum_i^{n_{reactions}} \nu_{ij} r_i$$

which reduces to the following for a single reaction

$$R_j = \nu_j r$$

For a gas phase problem we express component concentrations using an equation of state for the total concentration and multiply it by the mole fractions. In a PFR, the mole fractions are related to the molar flowrates. For this specific example the mole fraction of propane is

$$y_p = \frac{N_p}{\sum_j^{n_{components}} N_j}$$

Generate an M-file to solve the set of initial value ODEs that describe this example and that will write the output to a postscript file. This output should plot the molar flowrate of C<sub>3</sub>H<sub>6</sub>, a dependent variable, versus the volume, the independent variable.