both induction and pumping are operative.[3] An example of complex coupling starts with the Sabatier reaction of Eqn. 17.31 with the goal of converting CO_2:

$$CO_{2(g)} + 4H_{2(g)} \rightleftarrows CH_{4(g)} + 2H_2O_{(g)} \qquad K_{a,900K} = 0.3101 \qquad 17.43$$

Consier the possibility that equilibrium conversion may be inproved by the methane pyrolysis reaction of Eqn. 17.35,

$$CH_{4(g)} \rightleftarrows C_{(s)} + 2H_{2(g)} \qquad K_{a,900K} = 3.546 \qquad 17.44$$

The $C_{(s)}$ will not be present in the gas phase, and $K_a = (y_{H_2}P)^2/(y_{CH_4}P)$ applying the principles that we will discuss in Section 17.14. Suppose we consider feeding H_2:CO_2 in a 2:1 ratio which is less than the stoichiometric H_2. However, Eqn. 17.44 will produce H_2 to pump Eqn. 17.43, and will remove some CH_4 to induce Eqn 17.43. Under the specified feed conditions at 900K and 2 bar, equibrium conversion of CO_2 is 28.1% if no pyrolyis occurs. If we promote pyrolysis in the same reactor, and add the second reaction, CO_2 conversion will increase to 34.9%. This illustrates the possibilities of coupling reactions, but the subtle effect may not justify the coupled system. Biology uses coupling extensively as illustrated by homework problem 18.15 which is delayed to introduce the concepts for biological standard states in Chapter 18.

17.12 ENERGY BALANCES FOR REACTIONS

We have previously introduced the energy balance in Section 3.6 and also discussed adiabatic reactors. In this section we consider that there may be a there is a maximum possible value of $\dot{\xi}$ (outlet conversion) due to chemical equilibrium. Equilibrium may affect both adiabatic and nonadiabatic reactors, but we cover adiabatic reactors, and the extension to nonadiabatic should be obvious with the inclusion of the heat term.

Adiabatic Reactors

The energy balance for a steady-state adiabatic flow reactor is given in Eqn. 3.53 on page 118. The variables T^{out} and $\dot{\xi}$ from the energy balance also appear in the equilibrium constraint that will govern maximum conversion. Earlier, in Chapter 3, we considered the reaction coordinate to be specified. However, in a reaction-limited adiabatic reactor, we must solve the energy balance together with the equilibrium constraint to simultaneously determine the maximum conversion and adiabatic outlet temperature. Using the energy balance from Eqn. 3.53, do the following.

1. Write the energy balance, Eqn 3.53. Calculate the enthalpy of the inlet components at T^{in}.
2. Guess the outlet temperature, T^{out}. Calculate the enthalpy of the outlet components at T^{out}.
3. Determine $\dot{\xi}$ at T^{out} using the chemical equilibrium constant constraint.
4. Calculate $\dot{\xi}\Delta H_R^o$ for this conversion.
5. Check the energy balance for closure.
6. If the energy balance does not close, go to step 2.

As you might expect, this type of calculation lends itself to numerical solution, such as the Solver in Excel.

3. O'Connell, J.M., Fernandez, E., Komives, C. July, 2010. NSF BioEMB Workshop on Thermodynamics, San Jose, CA.