PROBLEM 14.49

KNOWN: CO at 77°F, 1 atm enters an insulated reactor operating at steady state and burns with air entering at 77°F, 1 atm. An equilibrium mixture of CO, CO₂, N₂ exits at 1 atm, T.

FIND: Determine T if the combustion occurs with 1.80% theoretical air, (a) 100% theoretical air.

SCHEMATIC & GIVEN DATA:

![Diagram of a reactor with CO and air inputs leading to a mixture output]

ANALYSIS: (a) The reaction of CO with 80% of theoretical air to form CO₂ and N₂ is described by

\[ \text{CO} + 0.40 \times 1.504 \text{ N}_2 \rightarrow x \text{ CO}_2 + (1-x) \text{ CO} + (0.8-0.2x) \text{ O}_2 + 1.504 \text{ N}_2 \]

The amount of mixture is \( n = x + (1-x) + (0.8-0.2x)/2 \). At equilibrium, CO ⇌ CO₂. According to Eq. 14.35, this form

\[ K(T) = \frac{[\text{CO}_2]^x}{[\text{CO}]^{1-x} [\text{O}_2]^{0.8-0.2x}} \]

Another equation relating \( x \) and \( T \) is obtained from an energy rate equation at steady state which reduces to give

\[ \frac{x}{0.4} \text{ h}_{\text{CO}} + 0.4 \text{ h}_{\text{O}_2} + 1.504 \text{ h}_{\text{N}_2} \rightarrow -[(x+1-x) \text{ h}_{\text{CO}} + (0.8-0.2x) \text{ h}_{\text{O}_2}] \]

Then, with \( h_{\text{N}_2} = 0 \) for \( \text{N}_2 \) and \( h_{\text{CO}} = h_{\text{CO}_2} \), this becomes

\[ 0 = [h_{\text{CO}}] x - [(x+1-x) h_{\text{CO}} + (0.8-0.2x) h_{\text{O}_2}] - [(h_{\text{CO}}) x + h_{\text{CO}_2}] - (0.2-0.2x) h_{\text{O}_2} + 1.504 \frac{h_{\text{N}_2}}{(577)}] \]

or with data from Table A-2.58

\[ x [\frac{h_{\text{CO}}}{h_{\text{CO}_2}} - 1.97] + (1-x) [\frac{h_{\text{CO}}}{h_{\text{N}_2}} - 1.337] + (0.2-0.2x) [\frac{h_{\text{O}_2}}{h_{\text{CO}_2}} - 773.1] + 1.504 [\frac{h_{\text{N}_2}}{(577)}] - 773.1] = -47.540 \]

For the products to include both CO and O₂, inspection of the reaction equation shows that \( x \) must be in the interval 0 < x < 0.8. Eqs. (1), (2) are simultaneous in \( x \) and \( T \). Solving iteratively with table data, \( T = 1980 \) K, \( x = 0.766 \).

(b) The reaction of CO with the theoretical amount of air to produce CO₂, CO, O₂, and N₂ is

\[ \text{CO} + \frac{1}{2} \text{ O}_2 + 1.88 \text{ N}_2 \rightarrow x \text{ CO} + (1-x) \text{ CO}_2 + \frac{x}{2} \text{ O}_2 + 1.88 \text{ N}_2 \]

For the products to include both CO and CO₂, \( x \) is necessary for \( x \) to be in the interval \( 0 < x < 1 \).

The amount of mixture is \( n = x + (1-x) + \frac{x}{2} + 1.88 = (0.764 + x)/2 \). At equilibrium, \( \text{CO} \leftrightarrow \text{CO}_2 \). Thus, Eq. 14.35 takes the form

\[ K(T) = \frac{[h_{\text{CO}}] x^{1/2} [h_{\text{CO}_2}^{0.8-0.2x}]}{[h_{\text{CO}}]^{1-x} [h_{\text{O}_2}]^{0.8-0.2x}} = \left( \frac{x}{1-x} \right)^{1/2} \left( \frac{x}{0.764+x} \right)^{1/2} \]

Continued on next slide
Problem 14-49 continued

Another equation involving $T_3$ and $x$ can be obtained from an energy rate balance which reduces at steady state to

$$0 = \frac{dQ}{dt} = \frac{W}{24} + \left[ 0.5 \bar{h}_{\text{N}_2} + 1.88 \bar{h}_{\text{N}_2} \right]_2 + \left[ \bar{h}_{\text{CO}} - x \bar{h}_{\text{CO}} + (1-x) \bar{h}_{\text{CO}_2} + \frac{x}{2} \bar{h}_{\text{O}_2} + 1.88 \bar{h}_{\text{N}_2} \right]_3$$

Then, with $T_f = 225$ for $O_2$ and $N_2$, this becomes

$$x \left[ \bar{h}_{\text{f}} + \bar{h}(T_f) - \bar{h}(298) \right]_{\text{CO}} + (1-x) \left[ \bar{h}_{\text{f}} + \bar{h}(T_f) - \bar{h}(298) \right]_{\text{CO}_2} + \frac{x}{2} \left[ \bar{h}(T_f) - \bar{h}(298) \right]_{\text{O}_2}$$

and

$$+ 1.88 \left[ \bar{h}(T_f) - \bar{h}(298) \right]_{\text{N}_2} = \left( \bar{h}_{\text{f}} \right)_{\text{CO}}$$

Noting that 225°F corresponds to 250°C, we use data from the SI Table A-23 to obtain

$$x \left[ -110,530 + \bar{h}(T_f) - 8669 \right]_{\text{CO}} + (1-x) \left[ -393,520 + \bar{h}(T_f) - 9364 \right]_{\text{CO}_2} + \frac{x}{2} \left[ \bar{h}(T_f) - 8682 \right]_{\text{O}_2}$$

$$+ 1.88 \left[ \bar{h}(T_f) - 8669 \right]_{\text{N}_2} = -110,530$$

or

$$x \left[ \bar{h}(T_f) - 110,530 \right]_{\text{CO}} + (1-x) \left[ \bar{h}(T_f) - 407,889 \right]_{\text{CO}_2} + \frac{x}{2} \left[ \bar{h}(T_f) - 8682 \right]_{\text{O}_2} + 1.88 \left[ \bar{h}(T_f) - 8669 \right]_{\text{N}_2}$$

$$= -110,530$$

Equations (1), (2) are simultaneous equations for $x$, $T_3$. Solving

(1) iteratively with table data, $x = 0.125$, $T_3 = 2399 K$ (4318°F)}
Problem 14-49 continued

IT can be used as an alternative to an iterative solution by hand using table data. The program follows.

**IT Code**

```
T1 = 77 + 459.67 // °R
T2 = 77 + 459.67 // °R
p3 = 1 // atm
ndotCO_1 = 1 // Do calculations on the basis of 1 lbmol of CO entering.

// CO + a (0.5) (O2 + 3.76 N2) → x CO2 + (1 - x) CO + ((1 - x) / 2) O2 + a 1.88 N2

ndotCO2_3 = x
ndotCO_3 = 1 - x
ndotO2_3 = (a - x) / 2
ndotN2_3 = a * 1.88
ndot_3 = ndotCO2_3 + ndotCO_3 + ndotO2_3 + ndotN2_3
yCO2 = ndotCO2_3 / ndot_3
yO2 = ndotO2_3 / ndot_3
yCO = ndotCO_3 / ndot_3
pref = 1 // atm
// Part (a):
a = 0.8
// For Part(b): Set a = 1.

// For the reaction CO2 <=>>> CO + 1/2 O2
K = ((xyCO) * (yO2)*0.5) / (yCO2)) * (p3 / pref)^ 5
// Data from Table A-27 are stored in EQCO2A.LUT.
log(K) = LOOKUPVAL(EQCO2A,2,T3,3)

0 = hCO_1 + a*0.5*hO2_2 + a*1.88*hN2_2 - x*hCO2_3 - (1-x)*hCO_3 -
   ((a-x)/2)*hO2_3 - a*1.88*hN2_3
hCO_1 = h_T("CO",T1)
hO2_2 = h_T("O2",T2)
hN2_2 = h_T("N2",T2)
hCO2_3 = h_T("CO2",T3)
hCO_3 = h_T("CO",T3)
hO2_3 = h_T("O2",T3)
hN2_3 = h_T("N2",T3)
```

**IT Results**

Part (a): 80% theoretical air: x = 0.7658, T3 = 4380°R

Part (b): Theoretical air: x = 0.8751 (lbmol of CO out per lbmol of CO in)
T3 = 4318°R