**14-4-1** [BSP] An equimolar mixture of carbon monoxide and water vapor at 1 atm and 298 K enters a reactor operating at steady state. The equilibrium mixture, composed of CO_2, CO, $H_2O(g)$ and H_2, leaves at 2000 K. Determine (a) equilibrium composition of CO_2 in the mixture, (b) the heat transfer (Q) between the reactor and surroundings in kJ per kmol of CO entering the reactor.

SOLUTION

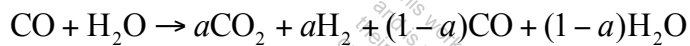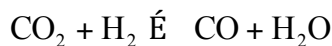First, we start with balancing the equation:

$$CO + H_2O \rightarrow aCO_2 + bH_2 + cCO + dH_2O$$
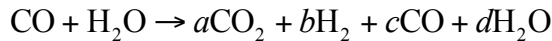
$$C : 1 = a + c \Rightarrow c = 1 - a$$
$$O : 2 = 2a + c + d \Rightarrow 2 = 2a + (1-a) + d \Rightarrow d = 1 - a$$
$$H_2 : 1 = b + d \Rightarrow a = b$$

$$CO + H_2O \rightarrow aCO_2 + aH_2 + (1-a)CO + (1-a)H_2O$$

Now we need one more equation. The equilibrium constant equation of the stoichiometric reaction of the products will be used to get this equation.

$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$

The equilibrium constant equation;

$$K = \left(\frac{y_{CO} y_{H_2O}}{y_{CO_2} y_{H_2}} \right) \left(\frac{1}{1} \right)^{2-2} = \frac{(1-a)(1-a)}{(a)(a)} = \frac{1-2a+a^2}{a^2}$$

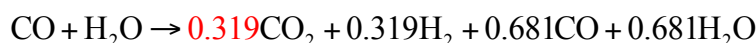From the equilibrium constant table we get
$$K = e^{1.51} = 4.53$$

Now we find a solving the following equation
$$4.53 = \frac{1-2a+a^2}{a^2};$$
$$\Rightarrow a = 0.319$$

So the balanced overall reaction will be
$$CO + H_2O \rightarrow 0.319CO_2 + 0.319H_2 + 0.681CO + 0.681H_2O$$

Now we can find the heat transfer using the energy balance equation;

$$\frac{\cancel{Q}}{\cancel{n}_F} = \bar{h}_P - \bar{h}_R$$

where, $\bar{h}_P$ and $\bar{h}_R$ can be evaluated using the procedure described in chapter 13.

$$\bar{h}_P = -230890.15 \frac{kJ}{kmol}$$

$$\bar{h}_R = -352154.57 \frac{kJ}{kmol}$$

Therefore,

$$\frac{\dot{Q}}{\dot{n}_F} = \bar{h}_P - \bar{h}_R = -230890.15 - (-352154.57) = 121264.42 \frac{kJ}{kmol\ CO}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-2 [BSX] Carbon dioxide gas at 1 atm, 298 K enters a reactor operating at steady state. If an equilibrium mixture of CO_2, CO and O_2 exits at 2800 K, 1 atm, determine (a) the composition of the CO_2 in the products and (b) the heat transfer to the surroundings per unit mass of carbon dioxide.
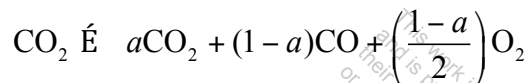
SOLUTION

Balancing the equation;
$$CO_2 \rightleftharpoons aCO_2 + bCO + cO_2$$
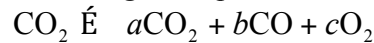
$$a + b = 1 \Rightarrow b = 1 - a$$

$$a + 2c = 1 \Rightarrow c = \frac{1-a}{2}$$

Balanced equation is

$$CO_2 \rightleftharpoons aCO_2 + (1-a)CO + \left(\frac{1-a}{2}\right)O_2$$

The exit mixture is assumed to be an equilibrium mixture, thus;

$$CO_2 \rightleftharpoons CO + \frac{1}{2}O_2$$

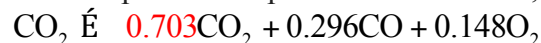$$y_{CO_2} = \frac{2a}{3-a}; \; y_{CO} = \frac{2(1-a)}{3-a}; \; y_{O_2} = \frac{1-a}{3-a}$$

The equilibrium constant equation

$$K = \left(\frac{y_{CO} y_{O_2}^{0.5}}{y_{CO_2}}\right)\left(\frac{p}{p_0}\right)^{1+0.5-1} = \left(\frac{2(1-a)}{3-a}\right)\left(\frac{1-a}{3-a}\right)^{0.5}\left(\frac{3-a}{2a}\right) \Rightarrow K = \frac{(1-a)}{a}\sqrt{\frac{1-a}{3-a}}$$

Using Table G-3 at 2800 K;
$$\Rightarrow e^{-1.894} = \frac{(1-a)}{a}\sqrt{\frac{1-a}{3-a}}$$
Solving, $a = 0.703$

The composition of products is therefore,
$$CO_2 \rightleftharpoons 0.703CO_2 + 0.296CO + 0.148O_2$$

(b) The heat transfer to the surroundings per unit mass of CO_2

$$\frac{\dot{Q}}{\dot{m}_F} = \bar{h}_P - \bar{h}_R$$

$$\bar{h}_P = -171886.61 \, \frac{\text{kJ}}{\text{kmol}}$$

$$\bar{h}_R = -393404.38 \, \frac{\text{kJ}}{\text{kmol}}$$

Therefore,

$$\frac{\dot{Q}}{\dot{n}_F} = \bar{h}_P - \bar{h}_R = -171886.61 - \left(-393404.38\right) = 221517.7 \, \frac{\text{kJ}}{\text{kmol CO}_2} = 5034.49 \, \frac{\text{kJ}}{\text{kg CO}_2}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-3 [BSC] Hydrogen is heated in an open-steady device at 100 kPa from 300 K to 3000 K at a rate of 0.5 kg/min. Determine the rate of heat transfer in kW, assuming (a) no dissociation takes place, (b) dissociation takes place.

SOLUTION

The mass flow rate is given

$$\dot{m} = 0.5\frac{kg}{min} = 0.008333\frac{kg}{s}$$

(a) No dissociation takes place,

$$H_2 \rightleftarrows H_2$$

The heat transfer is

$$\dot{Q} = \dot{n}_F\left(\bar{h}_P - \bar{h}_R\right) = \dot{m}\left(h_P - h_R\right)$$

From the n-IGE Model Chemical Equilibrium TESTcalc

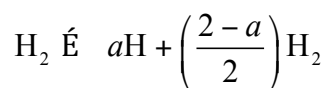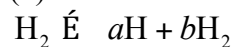$$h_P = 44019.21\frac{kJ}{kg}$$

$$\bar{h}_R = 26.57\frac{kJ}{kg}$$

Therefore,

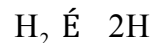$$\dot{Q} = \dot{m}\left(h_P - h_R\right) = (0.008333)(44019.21 - 26.57) = 366.6 \text{ kW}$$

(b) Dissociation takes place,

$$H_2 \rightleftarrows aH + bH_2$$

$$H_2 \rightleftarrows aH + \left(\frac{2-a}{2}\right)H_2$$

The exit mixture is assumed to be an equilibrium mixture, thus;

$$H_2 \rightleftarrows 2H$$

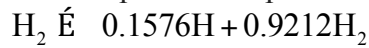$$y_H = \frac{2a}{a+2}; \ y_{H_2} = \frac{2-a}{a+2}$$

The equilibrium constant equation;

$$K = \frac{y_H^2}{y_{H_2}} = \frac{4a^2}{(a+2)^2}\frac{a+2}{2-a} \Rightarrow K = \frac{4a^2}{4-a^2}$$

Using Table G-3 at 3000 K

$$\Rightarrow \quad e^{-3.685} = \frac{4a^2}{4 - a^2}$$

Solving, $a = 0.1576$

The composition of products is therefore,

$H_2 \acute{E} \quad 0.1576 H + 0.9212 H_2$

The heat transfer is

$$\dot{Q} = \dot{n}_F \left(\bar{h}_P - \bar{h}_R \right) = \dot{n} \left(h_P - h_R \right)$$

From the n-IGE Model Chemical Equilibrium TESTcalc

$$h_P = 61976.74 \frac{kJ}{kg}$$

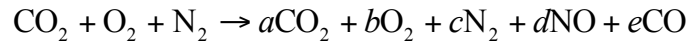$$\bar{h}_R = 26.57 \frac{kJ}{kg}$$

Therefore,

$$\dot{Q} = \dot{n} \left(h_P - h_R \right) = (0.008333)(61976.74 - 26.57) = 516.23 \, \text{kW}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis, IGE mixture model to verify the solution.

14-4-4 [BSV] An equimolar mixture of CO_2, O_2, and N_2 enter a reactor operating at steady state. An equilibrium mixture of CO_2, O_2, N_2, NO, and CO exits at 3500 K and 600 kPa. Determine the (a) molar amount of CO_2 (in kmols) in the mixture and (b) heat transfer (q) to the surroundings per unit mass of CO_2. Assume the surroundings to be 300 K and 100 kPa.
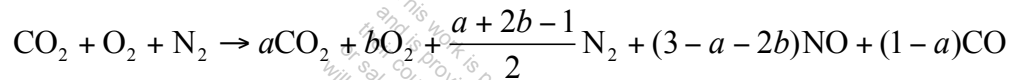
SOLUTION

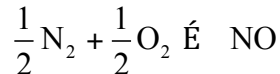First, we start with balancing the equation:

$$CO_2 + O_2 + N_2 \rightarrow aCO_2 + bO_2 + cN_2 + dNO + eCO$$

$$a + e = 1 \Rightarrow e = 1 - a$$
$$2c + d + = 2 \Rightarrow d = 2 - 2c$$
$$2a + 2b + d + e = 4 \Rightarrow a + 2b - 2c = 1$$

$$CO_2 + O_2 + N_2 \rightarrow aCO_2 + bO_2 + \frac{a + 2b - 1}{2}N_2 + (3 - a - 2b)NO + (1 - a)CO$$

At equilibrium two independent reactions relate the components of the mixture;

$$CO_2 \rightleftharpoons CO + \frac{1}{2}O_2$$

$$\frac{1}{2}N_2 + \frac{1}{2}O_2 \rightleftharpoons NO$$

For the first reaction

$$K_1 = \left(\frac{y_{CO} y_{O_2}^{0.5}}{y_{CO_2}} \right) \left(\frac{p}{p_0} \right)^{1+0.5-1} \Rightarrow \left(\frac{2(1-a)}{7-a} \right) \sqrt{\frac{2b}{7-a}} \left(\frac{7-a}{a} \right) \left(\frac{600}{100} \right)^{0.5} = e^{0.435}$$

For the second reaction;

$$K_2 = \left(\frac{y_{NO}}{y_{N_2}^{0.5} y_{O_2}^{0.5}} \right) \left(\frac{p}{p_0} \right)^{1-0.5-0.5} \Rightarrow \left(\frac{2(3-a-2b)}{7-a} \right) \sqrt{\frac{7-a}{a+2b-1}} \sqrt{\frac{2b}{7-a}} = e^{-1.601}$$

Solving two equations above
$a = 0.481$; $b = 1.155$

The heat transfer is;

$$\frac{\dot{Q}}{\dot{m}_F} = \bar{h}_P - \bar{h}_R$$

$$\overline{h}_P = 178722.9 \frac{\text{kJ}}{\text{kmol}}$$

$$\overline{h}_R = -393415.8 \frac{\text{kJ}}{\text{kmol}}$$

$$\overline{q} = \frac{\cancel{\dot{Q}}}{\cancel{\dot{n}_F}} = \overline{h}_P - \overline{h}_R = 178722.9 - \left(-393415.8\right) = 572138.7 \frac{\text{kJ}}{\text{kmol CO}_2}$$

Therefore,

$$q = \frac{\overline{q}}{\overline{M}_{\text{CO}_2}} = \frac{572138.7}{44} = 13003.15 \frac{\text{kJ}}{\text{kg CO}_2}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.
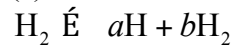
14-4-5 [BSQ] Hydrogen (H_2) is heated during a steady-flow process at 1 atm from 298 K to 3000 K at a rate of 0.6 kg/min. Determine the rate of heat transfer needed during this process, assuming (a) some H_2 dissociates into H and (b) no dissociation takes place.
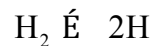
SOLUTION

The mass flow rate is given

$$\dot{m} = 0.6\,\frac{kg}{min} = 0.01\,\frac{kg}{s}$$

(a) Dissociation takes place,
$$H_2 \rightleftharpoons aH + bH_2$$
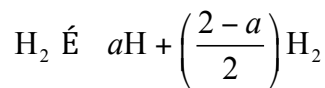
$$H_2 \rightleftharpoons aH + \left(\frac{2-a}{2}\right)H_2$$

The exit mixture is assumed to be an equilibrium mixture, thus;
$$H_2 \rightleftharpoons 2H$$

$$y_H = \frac{2a}{a+2}; \quad y_{H_2} = \frac{2-a}{a+2}$$
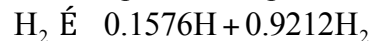
The equilibrium constant equation

$$K = \frac{y_H^{\,2}}{y_{H_2}} = \left(\frac{4a^2}{(a+2)^2}\right)\left(\frac{a+2}{2-a}\right) = \frac{4a^2}{4-a^2}$$

Using Table G-3 at 3000 K
$$\Rightarrow \quad e^{-3.685} = \frac{4a^2}{4-a^2}$$
Solving, $a = 0.1576$

The composition of products is therefore,
$$H_2 \rightleftharpoons 0.1576H + 0.9212H_2$$

The heat transfer is
$$\dot{Q} = \dot{n}_F\left(\bar{h}_P - \bar{h}_R\right) = \dot{m}\left(h_P - h_R\right)$$

From the n-IGE Model Chemical Equilibrium TESTcalc
$$h_P = 61859.70\,\frac{kJ}{kg}$$

$$\bar{h}_R = -2.05\,\frac{kJ}{kg}$$

Therefore,

$$\dot{Q} = \dot{m}(h_P - h_R) = (0.01)(61859.70 + 2.05) = 618.62 \text{ kW}$$

(b) No dissociation takes place,

$$H_2 \rightleftharpoons H_2$$

The heat transfer is

$$\dot{Q} = \dot{m}_F \left(\bar{h}_P - \bar{h}_R\right) = \dot{m}(h_P - h_R)$$
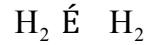
From the n-IGE Model Chemical Equilibrium TESTcalc

$$h_P = 44019.21 \frac{\text{kJ}}{\text{kg}}$$

$$\bar{h}_R = -2.05 \frac{\text{kJ}}{\text{kg}}$$

Therefore,

$$\dot{Q} = \dot{m}(h_P - h_R) = (0.01)(44019.21 + 2.05) = 440.2 \text{ kW}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis, IGE mixture model to verify the solution.

14-4-6 [BST] Carbon at 300 K, 100 kPa enters a chamber and reacts with oxygen entering at the same molar flow rate at 400 K, 100 kPa. An equilibrium mixture consists of CO_2, CO, and O_2 exits at 3000 K, 100 kPa. Determine the heat transfer to the surroundings in kJ/kmol of carbon.

SOLUTION

Molar analysis:
$$C + O_2 \rightarrow aCO_2 + bCO + cO_2$$

$$C: 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$O: 2 = 2a + b + 2c; \quad \Rightarrow c = \frac{1-a}{2}$$

Using the n-IGE Model TESTcalc, the coefficients are found to be
$$CO_2: \ a = 0.5615$$
$$CO: \ b = 0.4385$$
$$O_2: \ c = 0.2193$$

Using the molar masses of carbon and oxygen and assuming one kmol of each reactant, the mass of each reactant can be found. The conservation of mass can also be applied to find the total mass of products.

$$\bar{M}_C = 12 \frac{kg}{kmol}$$

$$\bar{M}_{O_2} = 32 \frac{kg}{kmol}$$

$$m_C = n_C \bar{M}_C = 12 \text{ kg}$$

$$m_{O_2} = n_{O_2} \bar{M}_{O_2} = 32 \text{ kg}$$

$$m_P = m_C + m_{O_2} = 12 + 32 = 44 \text{ kg}$$

Now using the n-IGE Model TESTcalc, the specific enthalpies of the reactants and products can be found

$$h_C = 59676.16 \frac{kJ}{kg}$$

$$h_{O_2} = 94.57 \frac{kJ}{kg}$$

$$h_P = -2571.29 \frac{kJ}{kg}$$

The energy equation can be used to find the heat transfer to the surroundings. Since there is no work done,

$$Q = m_P h_P - \sum \left(m_r h_r \right) = m_P h_P - \left(m_C h_C + m_{O_2} h_{O_2} \right);$$

$$Q = \left(44\right)\left(-2571.29\right) - \left[\left(12\right)\left(59676.16\right) + \left(32\right)\left(94.57\right)\right] = -832276.92 \text{ kJ} = -832.23 \text{ MJ}$$

$$Q_{out} = 832.23 \text{ MJ}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-7 [BSY] Steam enters a heat exchanger operating at steady state. An equilibrium mixture of H_2O, H_2, O_2, H, and OH exits at 2500 K and 100 kPa. Determine the (a) equilibrium composition of H_2O (in kmols) and (b) heat transfer (q) to the surroundings per unit mass of steam. Assume the surroundings to be 300 K and 100 kPa.
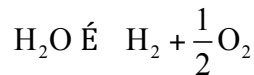
SOLUTION

Molar analysis:
$$H_2O \rightarrow aH_2O + bH_2 + cO_2 + dOH + eH$$
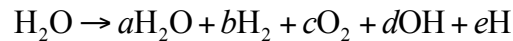
$$H:\ 2 = 2a + 2b + d + e$$
$$O:\ 1 = a + 2c + d$$

There are three reactions occurring simultaneously

$$H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2$$

$$H_2O \rightleftharpoons \frac{1}{2}H_2 + OH$$

$$H_2 \rightleftharpoons 2H$$
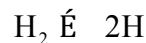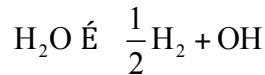
Using Table G-3, you get for the first, second, and third reactions, respectively
$$\ln K_{p,1} = -4.919$$
$$\ln K_{p,2} = -4.954$$
$$\ln K_{p,3} = -7.364$$

Using a different form of the relation for the equilibrium constant

$$\ln K_{p,1} = \ln\left[\left(\frac{N_{H_2}^{\nu_{H_2}} N_{O_2}^{\nu_{O_2}}}{N_{H_2O}^{\nu_{H_2O}}}\right)\left(\frac{p}{N_{total}}\right)^{\nu_{H_2} + \nu_{O_2} - \nu_{H_2O}}\right];$$

$$\Rightarrow -4.919 = \ln\left[\left(\frac{(b)(c)^{0.5}}{a}\right)\left(\frac{1}{a+b+c+d+e}\right)^{0.5}\right]$$

$$\ln K_{p,2} = \ln\left[\left(\frac{N_{H_2}^{\nu_{H_2}} N_{OH}^{\nu_{OH}}}{N_{H_2O}^{\nu_{H_2O}}}\right)\left(\frac{p}{N_{total}}\right)^{\nu_{H_2} + \nu_{OH} - \nu_{H_2O}}\right];$$

$$\Rightarrow -4.954 = \ln\left[\left(\frac{(b)^{0.5}(d)}{a}\right)\left(\frac{1}{a+b+c+d+e}\right)^{0.5}\right]$$

$$\ln K_{p,3} = \ln\left[\left(\frac{N_H^{\nu_H}}{N_{H_2}^{\nu_{H_2}}}\right)\left(\frac{p}{N_{total}}\right)^{\nu_H - \nu_{H_2}}\right];$$

$$\Rightarrow -7.364 = \ln\left[\left(\frac{(e)^2}{b}\right)\left(\frac{1}{a+b+c+d+e}\right)^1\right]$$

Now with five equations and five unknowns, the coefficients can be found. Using the n-IGE Model Chemical Equilibrium TESTcalc, the coefficients are

H_2O : $a = 0.9403$

H_2 : $b = 0.0438$

O_2 : $c = 0.0167$

OH : $d = 0.0262$

H : $e = 0.0053$

Using the n-IGE Model Chemical Equilibrium TESTcalc, the following enthalpies are obtained

$$h_P = -6935.37 \frac{kJ}{kg}$$

$$h_R = -13419.10 \frac{kJ}{kg}$$

Since there is no work, the energy equation will be

$$Q = m(h_P - h_R) = 1(-6935.37 + 13419.10) = 6483.73 \frac{kJ}{kg\ H_2O}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-8 [BSJ] Propane gas (C_3H_8) at 300 K and 100 kPa enters combustion chamber operating at steady state and reacts with 100% of excess air entering at 350 K and 100 kPa. An equilibrium mixture consists of CO_2, CO, H_2O(g), H_2, O_2, and N_2 exits at 1100 K and 100 kPa. Determine (a) the heat transfer (Q) to the surroundings in kJ/kmol of propane. (b) What-if Scenario: What would the heat transfer be if 200% excess air enters the chamber instead?

SOLUTION
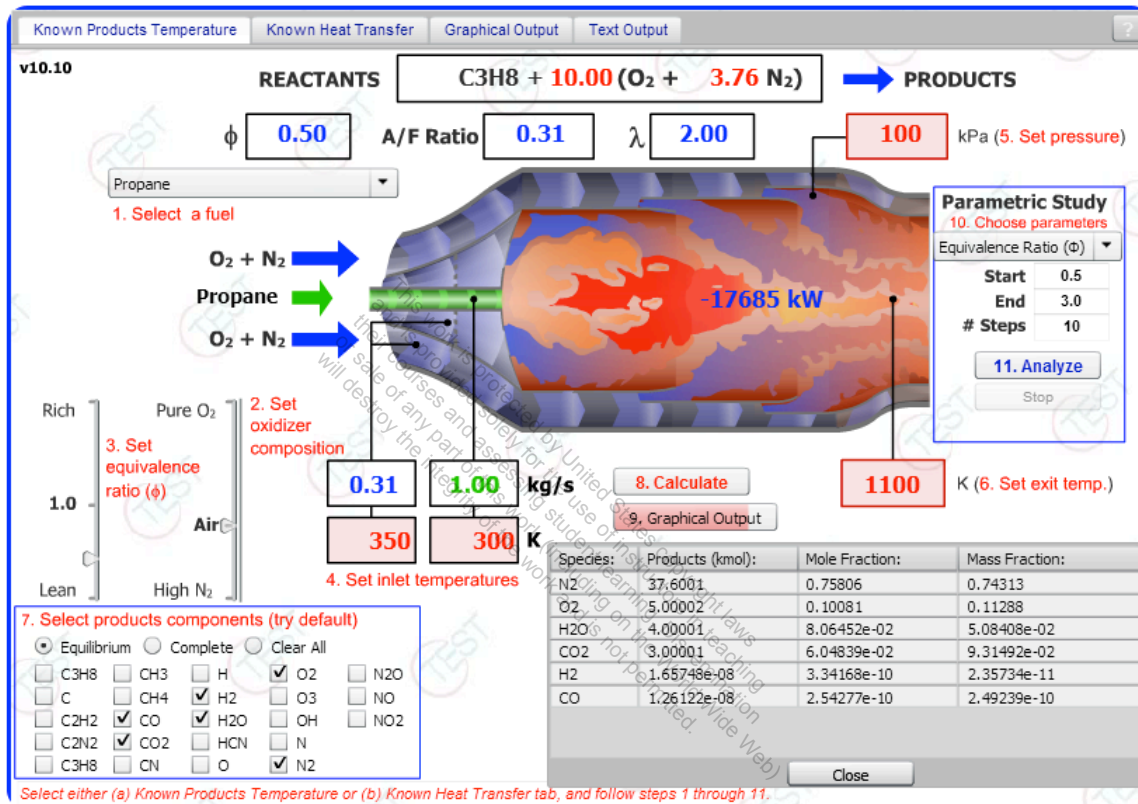
The heat transfer per kmol of propane

$$\bar{q} = q\bar{M}_{C_3H_8} = (-17685)(44.1) = -779908.5 \frac{kJ}{kmol\ C_3H_8}$$

$$\bar{q}_{out} = 779908.5 \frac{kJ}{kmol\ C_3H_8}$$

14-4-9 [BSF] Methane gas (CH_4) at 300 K and 100 kPa enters combustion chamber operating at steady state and reacts with 50% of excess air entering at 400 K and 100 kPa. An equilibrium mixture of CO_2, CO, $H_2O(g)$, H_2, and N_2 exits at 2000 K and 100 kPa. Determine (a) the heat transfer (Q) to the surroundings in kJ/kmol of methane. (b) What-if Scenario: What would the heat transfer be if 100% excess air enters the chamber instead?

SOLUTION
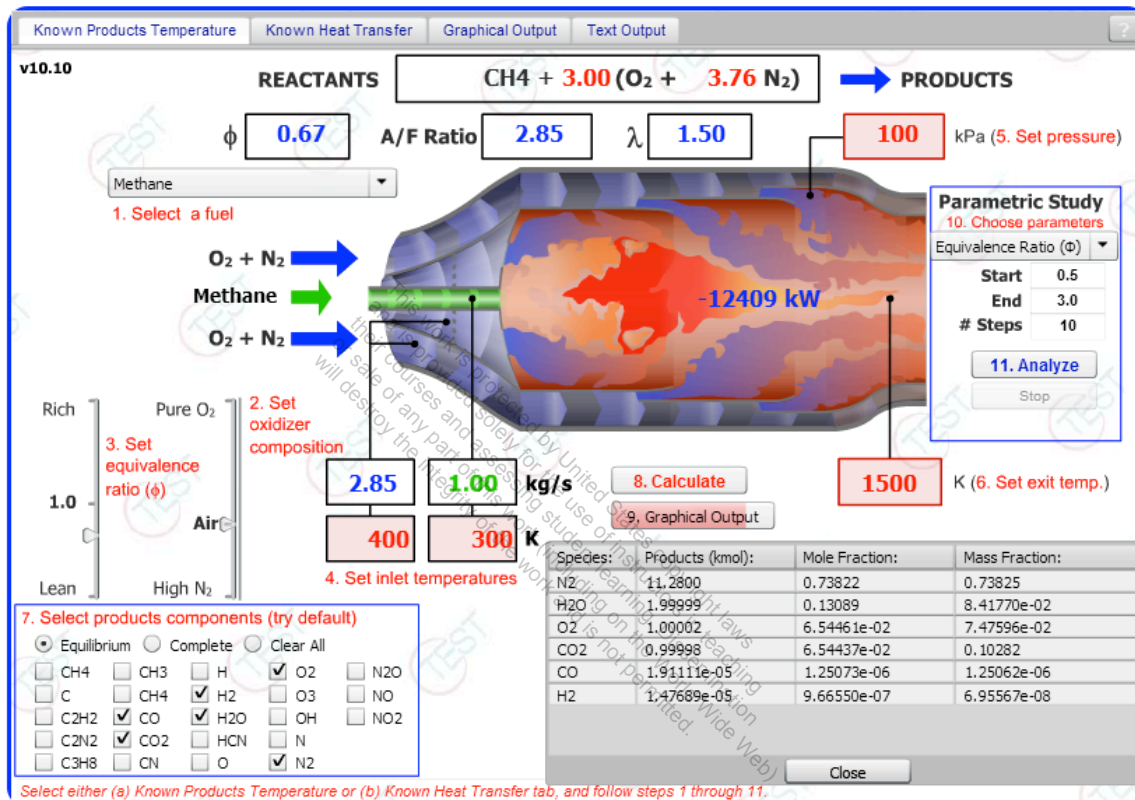
The heat transfer per kmol of methane

$$\bar{q} = q\bar{M}_{CH_4} = (-12409)(16) = -198544 \frac{kJ}{kmol\ CH_4}$$

$$\bar{q}_{out} = 198544 \frac{kJ}{kmol\ CH_4}$$

14-4-10 [BSD] CO_2 gas at 300 K and 400 kPa enters a steady state heat exchanger. An equilibrium mixture consists of CO_2, O_2, and CO exits at 2700 K and 350 kPa. Determine the (a) composition of CO_2 in the exiting mixture and (b) heat transfer (Q) to the gas in kJ/kmol of CO_2.

SOLUTION

Molar analysis:
$$CO_2 \rightarrow aCO_2 + bCO + cO_2$$
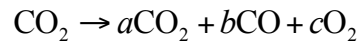
$$C: \quad 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$O: \quad 2 = 2a + b + 2c; \quad \Rightarrow c = \frac{1-a}{2}$$

$$a + b + c = \frac{3-a}{2}$$

$$y_{CO_2} = \frac{2a}{3-a}; \quad y_{CO} = \frac{2-2a}{3-a}; \quad y_{O_2} = \frac{1-a}{3-a}$$

Plugging the relations for the stoichiometric coefficients into the equation above we get,

$$CO_2 \rightarrow aCO_2 + (1-a)CO + \left(\frac{1-a}{2}\right)O_2$$
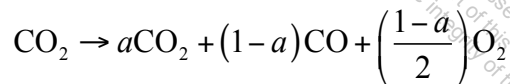
For $CO_2 \rightleftharpoons CO + \frac{1}{2}O_2$ use of the n-IGE Chemical Equilibrium TESTcalc finds at 2700 K and 350 kPa, $\ln K_p = -2.323$.

$$\ln K_p = \ln\left[\left(\frac{y_{CO}^{\nu_{CO}} y_{O_2}^{\nu_{O_2}}}{2 \, y_{CO_2}^{\nu_{CO_2}}}\right)\left(\frac{p}{p_0}\right)^{\nu_{CO}+\nu_{O_2}-\nu_{CO_2}}\right] = \ln\left[\left(\frac{y_{CO}^1 y_{O_2}^{0.5}}{y_{CO_2}^1}\right)(3.5)^{1.5-1}\right] = \ln\left[\frac{\left(\frac{2-2a}{3-a}\right)^1 \left(\frac{1-a}{3-a}\right)^{0.5}}{\left(\frac{2a}{3-a}\right)^1}(3.5)^{0.5}\right];$$

$$\ln K_p = \ln\left[\left(\frac{2-2a}{2a}\right)\left(\frac{p}{3-a}\right)^{0.5}(3.5)^{0.5}\right]; \quad \Rightarrow -2.323 = \ln\left[\left(\frac{1-a}{a}\right)\left(\frac{1-a}{3-a}\right)^{0.5}(3.5)^{0.5}\right];$$

$$\Rightarrow e^{-2.323} = \left[\left(\frac{1-a}{a}\right)\left(\frac{1-a}{3-a}\right)^{0.5}(3.5)^{0.5}\right]; \quad \Rightarrow 0.09797921 = \left[\left(\frac{1-a}{a}\right)\left(\frac{1-a}{3-a}\right)^{0.5}(3.5)^{0.5}\right];$$

$$\Rightarrow 0.00959993 = \left[\left(\frac{1-a}{a}\right)^2\left(\frac{1-a}{3-a}\right)(3.5)\right]; \quad \Rightarrow 0.00274284 = \left[\frac{1-3a+3a^2-a^3}{3a^2-a^3}\right]$$

Solving yields
$a = 0.8390$

Therefore

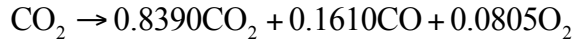$CO_2: \; a = 0.8390$

$CO: \; b = 1 - a = 1 - 0.8390 = 0.1610$

$O_2: \; c = \dfrac{1-a}{2} = \dfrac{1 - 0.8390}{2} = 0.0805$

Substituting in the known values

$$CO_2 \rightarrow 0.8390\,CO_2 + 0.1610\,CO + 0.0805\,O_2$$

Using the n-IGE Model Chemical Equilibrium TESTcalc, the following enthalpies are obtained

$$h_P = -215084.80 \,\frac{kJ}{kg}$$

$$h_R = -393330.44 \,\frac{kJ}{kg}$$

Using the molar mass of carbon dioxide and knowing that mass is conserved,

$$\bar{M}_{CO_2} = 44 \,\frac{kg}{kmol}$$

$$m_1 = m_2 = n\bar{M}_{CO_2} = (1)(44) = 44 \,\frac{kg}{kmol\,CO_2}$$

Since there is no work, the equation will be

$$Q = m_2 h_P - m_1 h_R = -215084.80 + 393330.44 = 178245.64 \,\frac{kJ}{kmol\,CO_2} = 178.25 \,\frac{MJ}{kmol\,CO_2}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-11 [BSM] Carbon monoxide at 20°C and 100 kPa enters a combustion chamber and burns with 25% excess air entering at the same temperature and pressure. An equilibrium mixture consists of CO_2, CO, O_2, and N_2 exits at 1200°C and 100 kPa. Determine (a) the heat transfer (Q) to the surroundings in kJ/kmol of CO. (b) What-if Scenario: What would the heat transfer to the surroundings be if 85% excess air enters the chamber instead?

SOLUTION

Molar analysis:

$$CO + 0.625(O_2 + 3.76N_2) \rightarrow aCO_2 + bCO + cO_2 + dN_2$$
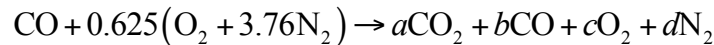
$$C: \; 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$O: \; 2.25 = 2a + b + 2c; \quad \Rightarrow c = \frac{1.25 - a}{2}$$

$$N: \; 2.35 = d$$

$$a + b + c + d = \frac{7.95 - a}{2}$$

$$y_{CO_2} = \frac{2a}{7.95 - a}; \quad y_{CO} = \frac{2 - 2a}{7.95 - a}; \quad y_{O_2} = \frac{1.25 - a}{7.95 - a}; \quad y_{N_2} = \frac{4.70}{7.95 - a}$$

Plugging the relations for the stoichiometric coefficients into the equation above we get,

$$CO + 0.625(O_2 + 3.76N_2) \rightarrow aCO_2 + (1 - a)CO + \left(\frac{1.25 - a}{2}\right)O_2 + 2.35N_2$$
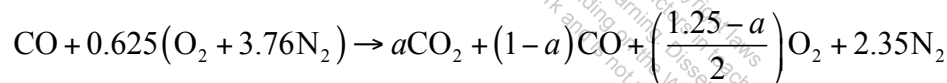
For $CO_2 \; \rightleftharpoons \; CO + \frac{1}{2}O_2$ use of the n-IGE Chemical Equilibrium TESTcalc finds at 1200°C, $\ln K_p = -12.635$. At 100 kPa,

$$\ln K_p = \ln\left[\left(\frac{y_{CO}^{\nu_{CO}} y_{O_2}^{\nu_{O_2}}}{y_{CO_2}^{\nu_{CO_2}}}\right)\left(\frac{p}{p_0}\right)^{\nu_{CO} + \nu_{O_2} - \nu_{CO_2}}\right] = \ln\left[\left(\frac{y_{CO}^1 y_{O_2}^{0.5}}{y_{CO_2}^1}\right)(1)^{1.5-1}\right] = \ln\left[\frac{\left(\frac{2-2a}{7.95-a}\right)^1\left(\frac{1.25-a}{7.95-a}\right)^{0.5}}{\frac{2a}{7.95-a}}\right];$$

$$\ln K_p = \ln\left[\left(\frac{2-2a}{2a}\right)\left(\frac{1.25-a}{7.95-a}\right)^{0.5}\right]; \quad \Rightarrow -12.635 = \ln\left[\left(\frac{1-a}{a}\right)\left(\frac{1.25-a}{7.95-a}\right)^{0.5}\left(\frac{2a}{7.95-a}\right)^1\right]$$

$$\Rightarrow e^{-12.635} = \left[\left(\frac{1-a}{a}\right)\left(\frac{1.25-a}{7.95-a}\right)^{0.5}\right]; \quad \Rightarrow 3.256 \times 10^{-6} = \left[\left(\frac{1-a}{a}\right)\left(\frac{1.25-a}{7.95-a}\right)^{0.5}\right];$$

$$\Rightarrow 1.060 \times 10^{-11} = \left[\left(\frac{1-a}{a}\right)^2\left(\frac{1.25-a}{7.95-a}\right)\right]; \quad \Rightarrow 1.060 \times 10^{-11} = \left[\frac{1.25 - 3.5a + 3.25a^2 - a^3}{7.95a^2 - a^3}\right];$$

$$\Rightarrow \left(1.060 \times 10^{-11}\right)\left(7.95a^2 - a^3\right) \cong 0 = 1.25 - 3.5a + 3.25a^2 - a^3;$$

$$\Rightarrow a = 1, \cancel{1.25}$$

The value of *a* cannot be above 1, otherwise the balance for carbon would demand a negative value for *b*.

Substituting in the known value for *a* yields
$$CO + 0.625\left(O_2 + 3.76N_2\right) \rightarrow CO_2 + 0.125O_2 + 2.35N_2$$
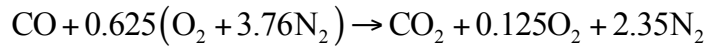
Now we can find the heat transfer using the energy balance equation;
$$Q - W_{ext} = \bar{h}_P - \bar{h}_R = \sum \nu_p \bar{h}_p - \sum \nu_r \bar{h}_r$$

Since there is no work, the equation will be;
$$Q = \sum \nu_p \bar{h}_p - \sum \nu_r \bar{h}_r = -231889 + 111119 = -120770 \frac{kJ}{kmol\ CO}$$

$$Q_{out} = 120770 \frac{kJ}{kmol\ CO}$$

	ν_k	$\bar{h}_f$	$\Delta\bar{h}_k$	$\bar{h}_k = \bar{h}_f + \Delta\bar{h}_k$	$\nu_k \bar{h}_k$
CO	1	-110530	-148	-110678	-110678
O₂	0.625	0	-148	-148	-93
N₂	2.35	0	-148	-148	-348
				$\sum \nu_r \bar{h}_r$	-111119
CO₂	1	-393520	67554	-325966	-325966
CO	0	-	-	-	0
O₂	0.125	0	48306	48306	6038
N₂	2.35	0	37465	37465	88042
				$\sum \nu_p \bar{h}_p$	-231886

Checking with the more accurate n-IGE Model TESTcalc,

$$Q_{out} = 129100 \frac{kJ}{kmol\ CO}$$

TEST Solution: Use TESTcalc Combustion and Chemical Equilibrium, Chemical Equilibrium Analysis to verify the solution.

14-4-12 [BSW] Methane (CH_4) at 25°C and 1 atm enters a well-insulated reactor and reacts with air entering at the same conditions. For steady-state operation, negligible effects of ke and pe, and negligible pressure loss, plot the temperature of the combustion products against equivalent ratio ranging from 0.5 through 3.0. (a) Assume complete combustion with PG mixture model, (b) assume complete combustion with IG mixture model, (c) assume equilibrium combustion with IG mixture model and having CO_2, H_2O, N_2, O_2, NO, OH, CO, O, H_2 and H in the products mixture. For part (c), also plot the mole fraction of CO and NO in the products against the equivalent ratio.

SOLUTION

The solution was done using TEST. But first, the equivalent ratio needed to be converted to the theoretical air percentage used, then to excess/deficit air percentage. The latter is a useful input in TEST.

$$\varphi = \frac{FA}{(FA)_{th}} = \frac{(AF)_{th}}{AF} = \frac{1}{x}, \text{ where x is the theoretical air percentage}$$

Then we get the excess/deficit percentage $= (x-1) \cdot 100$

The sign will tell whether it is excess (+) or deficit (-), the value can be plugged in TEST.

For example, $\varphi = 0.9$; $x = \frac{1}{\varphi} = \frac{1}{0.9} = 1.11$

The excess/deficit percentage $= (x-1) \cdot 100 = (1.11-1) \cdot 100 = 11\%$ excess
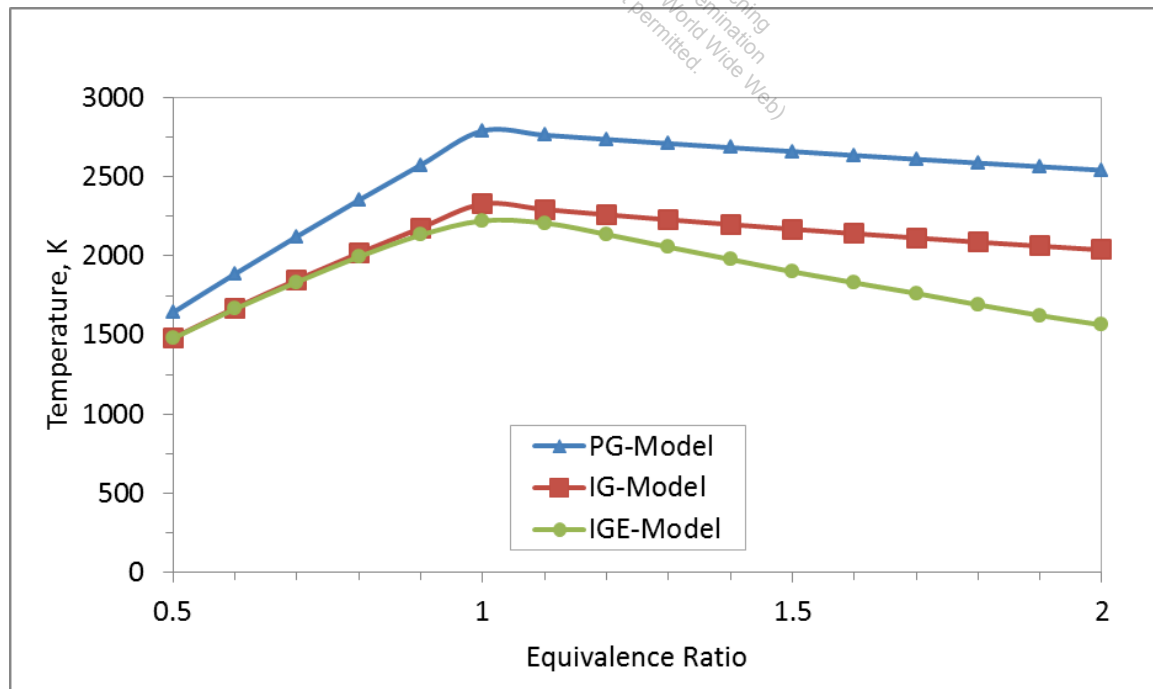
To compare the adiabatic flame temperature of the three different models used, they were plotted all in one graph.
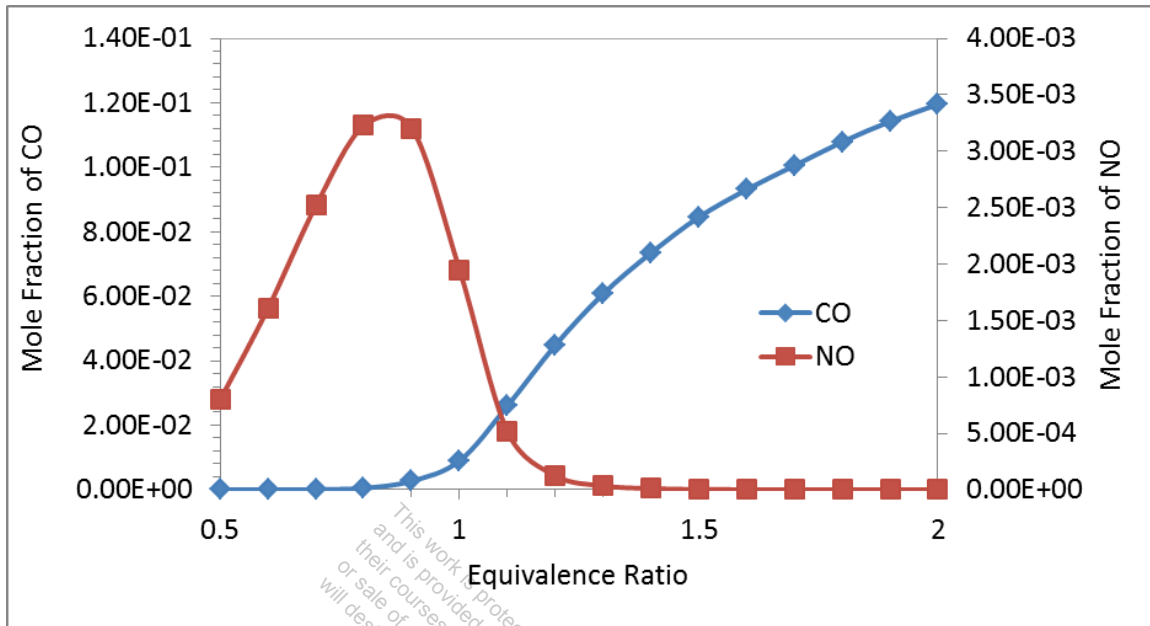
14-4-13 [BAR] Repeat 14-4-12[BSW] if the reactants enter the chamber at 800°C and 1 atm.

SOLUTION

The data for the plots below is collected using TEST.
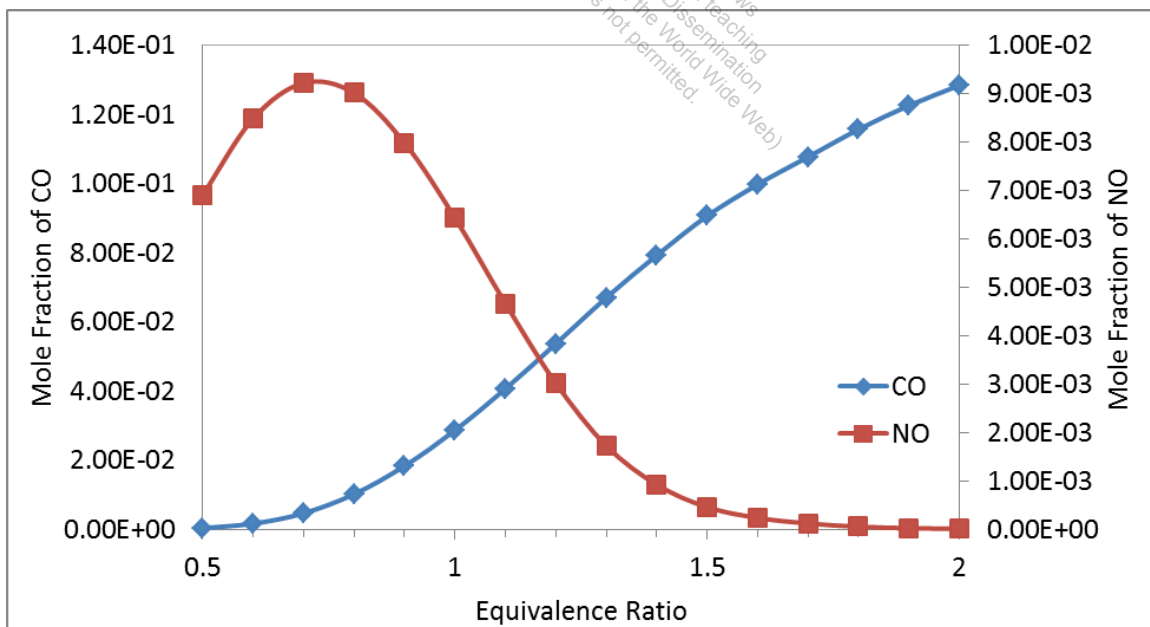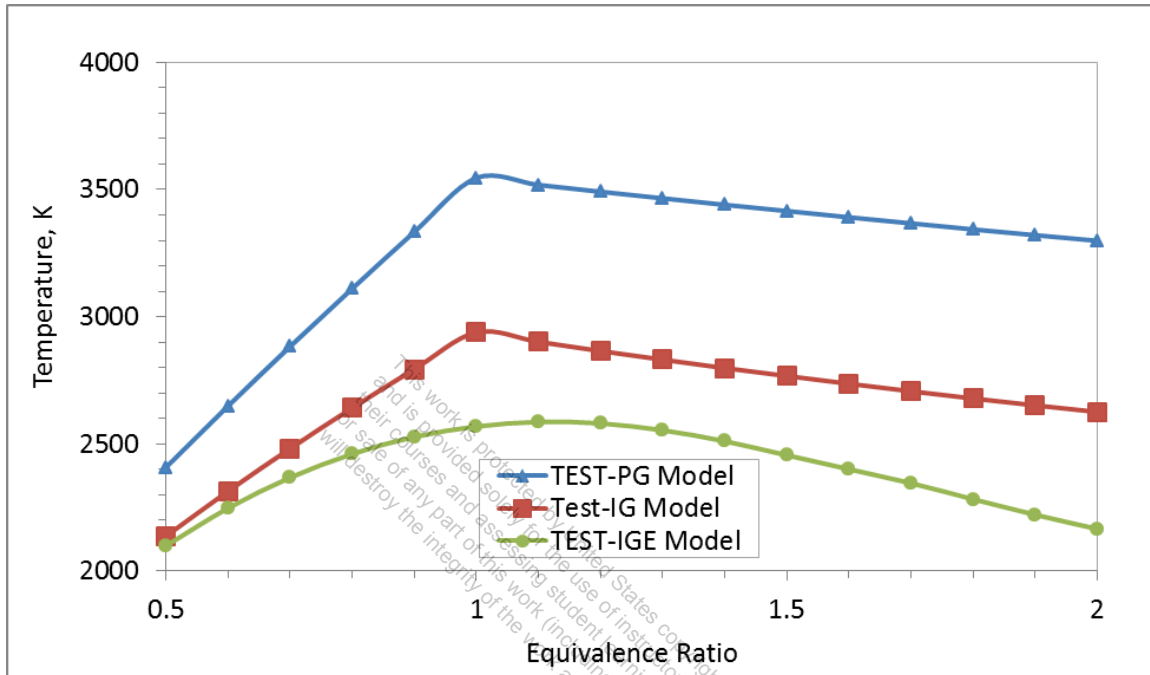
14-4-14 [BAO] Repeat 14-4-12[BSW] if the reactants enter the chamber at 600°C and 10 atm.

SOLUTION

The data for the plots below is collected using TEST.
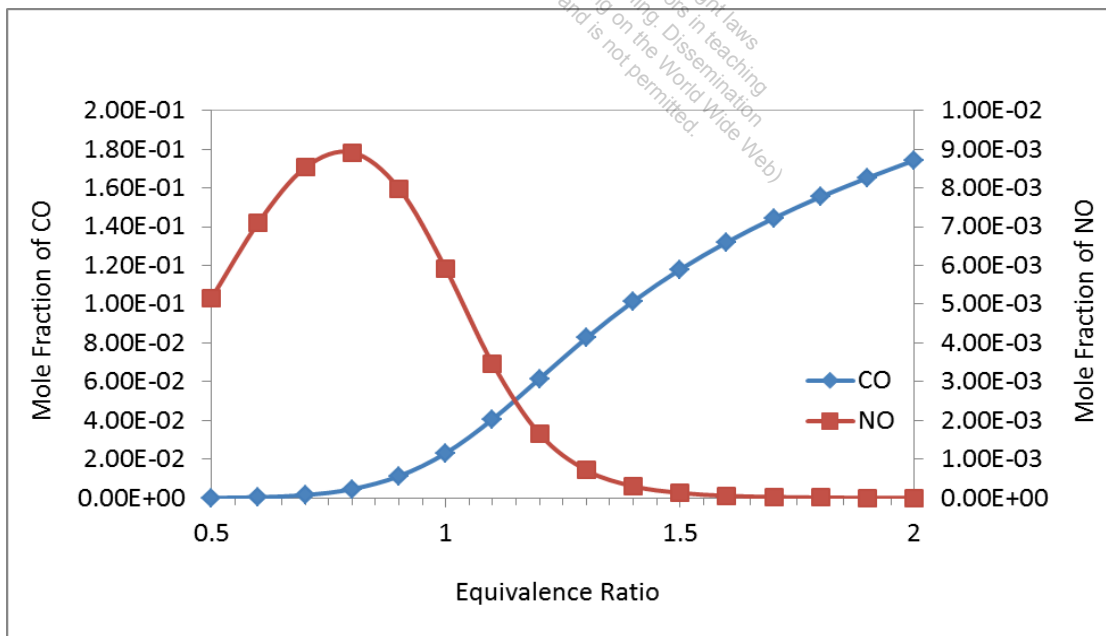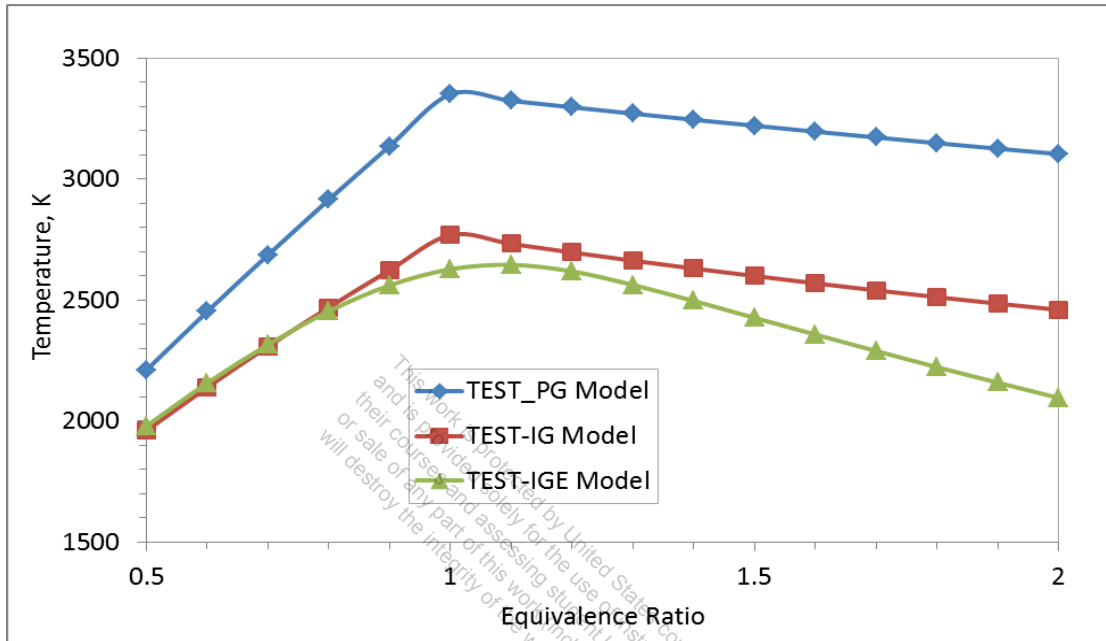
14-4-15 [BAB] Octane (C_8H_{18}) at 25°C, 1 atm enters a combustion chamber and reacts with 111% theoretical air entering at the same conditions. If the products exiting at 1800 K contains CO, CO_2, CN, H, H_2, H_2O, HCN, O, O_2, O_3, OH, N, N2, N_2O, NO and NO_2, determine (a) the molar fraction of NO in the products, in ppm and (b) the heat transfer rate for a fuel mass flow rate of 1 kg/s. (c) What-if Scenario: What would the molar fraction of NO be if the chamber were adiabatic? (d) What is the equilibrium flame temperature?

SOLUTION

14-4-16 [BVL] Octane (C_8H_{18}) at 25°C and 100 kPa enters a combustion chamber and reacts with 100% theoretical air entering at the same conditions. Determine the equilibrium flame temperature assuming the products contains CO, CO_2, CN, H, H_2, H_2O, HCN, O, O_2, O_3, OH, N, N2, N_2O, NO and NO_2. Use the equilibrium Interactive linked from the left margin. (c) What-if Scenario: How would the temperature change if the chamber pressure were increased to 1 MPa?

SOLUTION

14-4-17 [BVD] In problem 13-2-10 [BVF], an equilibrium mixture consisting of CO_2, CO, H_2, H_2O and O_2 exits at 2500 K, 100 kPa. Determine (a) molar composition of CO_2 at equilibrium and (b) the amount of heat transfer per kg of fuel. (c) What-if Scenario: What would be the heat transfer if there is no CO present in the products mixture?

SOLUTION

TEST Analysis Launch the open-steady IGE equilibrium TESTcalc. In the composition panel, compose the reactants (fuel and oxygen). Select the products components. Evaluate the reactants state, State-1, with p1 = 100 kPa, T1 = 298 K, and the products state, State-2, with p2 = p1 and T2 = 3000 K (select the Products radio-button). The mole fraction of CO2 can be found in the composition and the I/O panel. To determine the heat transfer, enter mdot1 = 478 kg/s, mdot2 = mdot1 (total amount of products for burning 1 kmol of fuel). In the device panel, load the inlet and exit states, and enter Wdot_ext = 0 to obtain Qdot, which is positive, indicating heat must be added to obtain the given exit temperature. Repeat the solution with no CO in the products.