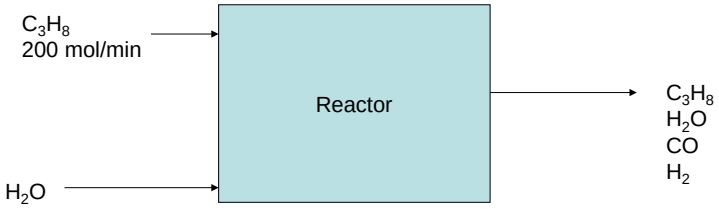
Molecular Species Balances with DOF Analysis



$$C_3H_8 + 3\ H_2O \rightarrow 3\ CO + 7\ H_2$$

DOF Analysis

Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2}	=	5
# of Rxns	=	+1
# of Species Balances	=	-4
# of Other Equations	=	0 → 2
Degrees of Freedom	=	2 → 0 (need to specify two things in order to solve problem)

Let's say that (a) there is 65% conversion of C_3H_8, and (b) there is 25% excess H_2O.

We now have 2 other equations, so the DOF = 0

$$X_i = \frac{n_0 - n}{n_0} = 1 - \frac{n}{n_0} \qquad n = n_0(1 - X_i)$$

A. Start with Conversion

$0.65 = 1 - n_{C3H8} / 200$ mol/min $\Rightarrow$ $n_{C3H8} = 200(1-0.65) = 70$ mol of C_3H_8/min

B. Now use the 25% excess H_2O

First find the stoichiometric amount of H_2O

$$(200\ mol/\min C_3H_8)\left(\frac{3\ moles\ H_2O}{mol\ C_3H_8}\right) = 600\ mol\ H_2O/min$$

With 25% excess, $n_{H2O,\ in}$ = (1.25)(600) = 750 mol H_2O/min

C. Now use species balances

$$n_{CO,out} = n_{CO,gen} = (n_{C3H8,cons})\left(\frac{\nu_{CO}\ moles\ CO\ formed}{\nu_{C_3H_8}\ moles\ C_3H_8\ consumed}\right)$$

200 − 70 =

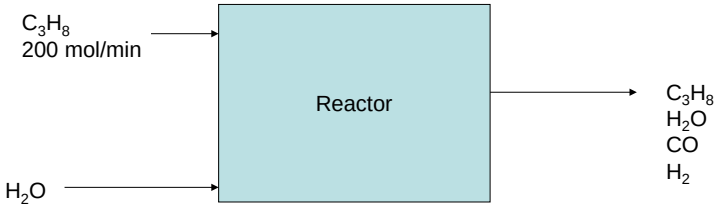
= 130 moles/min C_3H_8 consumed $\left(\frac{3}{1}\right)$ = 390 mol/min CO

$$n_{H2} = (n_{C3H8,cons})\left(\frac{7\ H_2\ gen}{mol\ C_3H_8\ cons}\right) = 130 \times 7 = 910 \text{ mol/min } H_2$$

$$n_{H2O,out} = n_{H2O,in} - n_{H2O,cons} = 750 - (130 \text{ mols } C_3H_8 \text{ cons})\left(\frac{3\ moles\ H_2O}{mol\ C_3H_8}\right) = 360 \text{ mol/min } H_2O$$

390

Atomic (Element) Balances with DOF Analysis



$$C_3H_8 + 3\ H_2O \rightarrow 3\ CO + 7\ H_2$$

DOF Analysis

Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2} = +5

Reacting elements = -3

Non Reacting Species = 0

# of Other Equations = 2 (Use 2 other equations from previous page)

Degrees of Freedom = 0

From fractional conversion and % Excess H2O, n_{C3H8} = 70 mol/min, $n_{H2O,in}$ = 750 mol/min

C Balance (in = out)

(200 mol C_3H_8/min)(3) = (70 mol C_3H_8/min)(3) + n_{CO} (1)

So n_{CO} = 600 − 210 = 390 mol CO/min

H Balance (in = out)

(200 mol C_3H_8/min)(8) + (750 mol H_2O/min)(2) =

(70 mol C_3H_8/min)(8) + n_{H2O} (2) + n_{H2}(2)

O Balance (in = out)

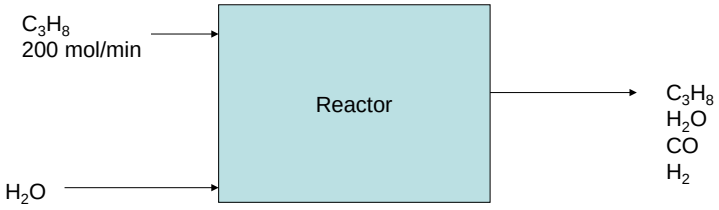
(750 mol H_2O/min)(1) = (390 mol CO/min)(1) + n_{H2O} (1)

So $n_{H2O,out}$ = 750 − 390 = 360 mol H_2O/min

Now go back to H balance:

$n_{H2,out}$ = $\frac{(1600 + 1500 - 560 - 720)}{2}$ = 910 $\frac{\text{mol } H_2}{\text{min}}$

Extent of Reaction Balances with DOF Analysis



$$C_3H_8 + 3\ H_2O \rightarrow 3\ CO + 7\ H_2$$

DOF Analysis

Unknowns: $n_{H2O,in}$, n_{C3H8}, n_{H2O}, n_{CO}, n_{H2}	= +5
Reactions	= -1
Reaction Species	= -4
Non Reacting Species	= 0
# of Other Equations	= -2 (Use 2 other equations from previous page)
Degrees of Freedom	= 0

From fractional conversion and % Excess H2O, n_{C3H8} = 70 mol/min, $n_{H2O,in}$ = 750 mol/min

70 200

$n_{C3H8} = n_{C3H8,in} + (-1)\xi$, so ξ = $(70 - 200)/(-1) = 130$ mol/min

$n_{H2O} = n_{H2O,in} + (-3)\xi$, so n_{H2O} = $750 - 3(130) = 360$ mol/min

$n_{H2} = n_{H2,in} + (7)\xi$, so n_{H2} = $7(130) = 910$ mol/min

$n_{CO} = n_{CO,in} + (3)\xi$, so n_{CO} = $3(130) = 390$ mol/min