ABSTRACT FOR STOICHIOMETRIC REACTOR

Description:

Stoichiometric reactor is used to get the composition of product stream given:

- Feed stream composition
- Coefficients of components involved in reaction
- Reaction Coordinate of each reaction

The important equations involved are:

$F_i = F_{i0} - (v_i/v_A) X_A F_{A0}$

X_A= Amount of limiting reagent converted/Amount of limiting reagent present in mixture just before reaction

Where, F_i is the molar flow rate of i^{th} component in product stream

F_{i0} is the molar flow rate of i^{th} component in feed stream

v_i is the stoichiometry of i^{th} component in reaction

v_A is the stoichiometry of limiting reagent in reaction

F_{A0} is the molar flow rate of limiting reagent in feed stream

Product compositions of reactions are calculated using sequential method and not simultaneously i.e. the code solves for the product composition after first reaction, and then uses this updated composition to find the product composition of next reaction.

Limiting Reagent is found by calculating the molar composition/stoichiometry ratio for reactants of a particular reaction. The reagent with least ratio is the limiting reagent.

References: http://www.iitg.ac.in/tamalb/documents/reactors.pdf

Examples:

1)Component System: CH_3CHO, CO, CH_4, O_2, CO_2

Thermodynamic Package: Peng Robinson/Lee Kesler

Reaction: $CH_3CHO \rightarrow CO + CH_4$ (Fractional conversion = 0.3)

$1/2O_2 + CO \rightarrow CO_2$ (Fractional conversion = 0.7)

Feed Composition: 0.5 moles O_2 and 0.5 moles CH_3CHO

Component	Method of Solving for number of moles	
	Analytical	DWSIM
CH_3CHO	0.35	0.34976363
CO	0.045	0.04496961
CH_4	0.15	0.1498987
O_2	0.4475	0.44719779
CO_2	0.105	0.10492909

2)Component System: CH_3CHO, CO, CH_4, O_2, CO_2

Thermodynamic Package: Soave-Redlich-Kwong (SRK)

Reaction: $CH_3CHO \rightarrow CO + CH_4$ (Fractional conversion = 0.3)

$1/2O_2 + CO \rightarrow CO_2$ (Fractional conversion = 0.7)

Feed Composition: 0.1 moles O_2 and 0.9 moles CH_3CHO

Component	Method of Solving for number of moles	
	Analytical	DWSIM
CH_3CHO	0.63	0.62930623
CO	0.13	0.12985684
CH_4	0.27	0.26970267
O_2	0.03	0.029966964
CO_2	0.14	0.13984583

3) Component System: C_2H_6, C_2H_4, H_2, C_2H_2
Thermodynamic Package: Soave-Redlich-Kwong (SRK)
Reaction: $C_2H_6 \rightarrow C_2H_4 + H_2$(Fractional conversion = 0.5)
$C_2H_6 \rightarrow C_2H_2 + 2H_2$(Fractional conversion = 0.7)
$C_2H_4 \rightarrow C_2H_2 + H_2$(Fractional conversion = 0.8)
Feed Composition: 0.6 moles C_2H_6, 0.5 moles H_2 and 0.9 moles C_2H_4

Component	Method of Solving for number of moles	
	Analytical	DWSIM
C_2H_6	0.09	0.0898025
C_2H_4	0.24	0.23947333
C_2H_2	1.17	1.1674325
H_2	1.22	2.1752161

4) Component System: C_2H_6, C_2H_4, H_2, C_2H_2
Thermodynamic Package: UNIFAC
Reaction: $C_2H_6 \rightarrow C_2H_4 + H_2$(Fractional conversion = 0.3)
$C_2H_6 \rightarrow C_2H_2 + 2H_2$(Fractional conversion = 0.2)
$C_2H_4 \rightarrow C_2H_2 + H_2$(Fractional conversion = 0.6)
Feed Composition: 0.4 moles C_2H_6, 0.9 moles H_2 and 0.1 moles C_2H_4

Component	Method of Solving for number of moles	
	Analytical	DWSIM
C_2H_6	0.224	0.22336457
C_2H_4	0.088	0.087750366
C_2H_2	0.188	0.18746669
H_2	1.254	1.2604143