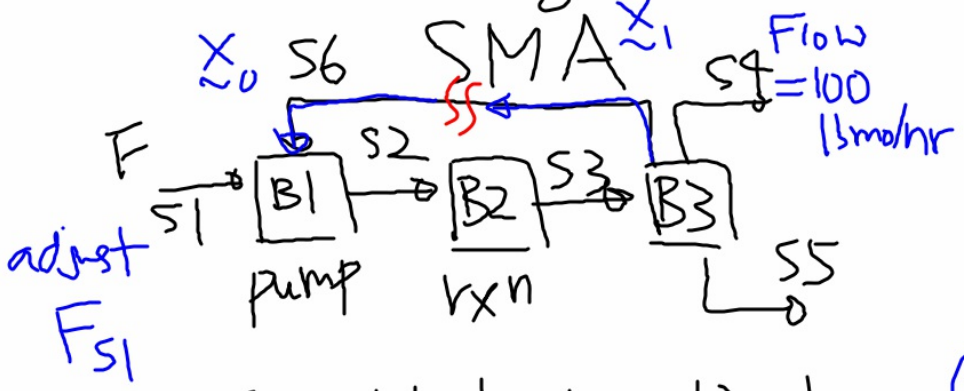
P.1) CHE 494 Friday Aug 18, 2023

iterate until $|\underset{\sim}{x}_0 - \underset{\sim}{x}_1| \leq$ tolerance

$11.2 \neq 11.2$ $10^{-4}$ or $10^{-6}$

$1 = 1$

steady-state process simulation ≡ flowsheeting




One block at a time!

Convergence

EBA/EOA

$\frac{dF}{dt} \quad \frac{dP}{dt} = 0$ $100 = 100$

model ≡ eqns $e^{x_1 x_2} - \ln x_1 = 10$

streams (lots of) $x_1^2 x_2 - \sin x_1^2 = 30$

simultaneously!

tear

S6 = recycle

Guess → $T, P, F_i$ ($N+2$ variables)

# of comps → $T, P$

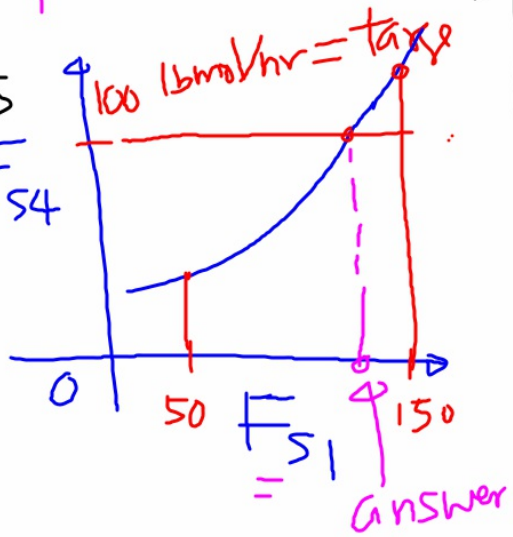
P.2

Convergence occurs: 20

(1) Recycles — ~~4~~ (N+2)*4 Tear streams

easier (2) Design targets

one var!




Input Data

Standard

Design targets (Design-specs)

(1) process feed T, P, $F_i$

$X_A$ in S6 = 0.99

(2) input for each block

At will allow only standard input

P.3) Use A+ to do mass-balance only

Feed → $F_i$

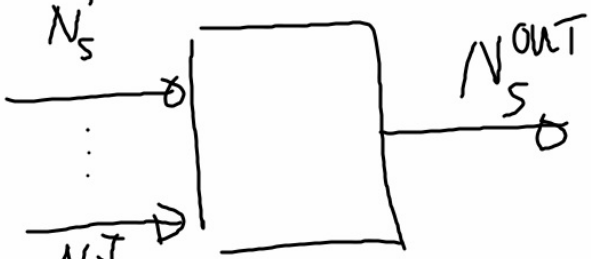
Blocks (elementary) modules

1) Mixer
2) Flow Splitter ←
3) Reactor
4) separator ←

pump
compressor

standard input:

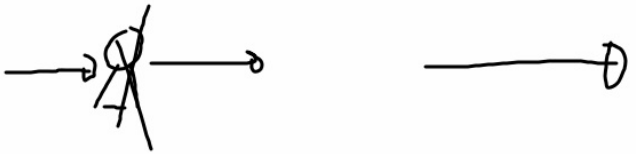
(1) Mixer




$$N_s^{OUT} = \sum_{i=1}^{J} N_s^i$$

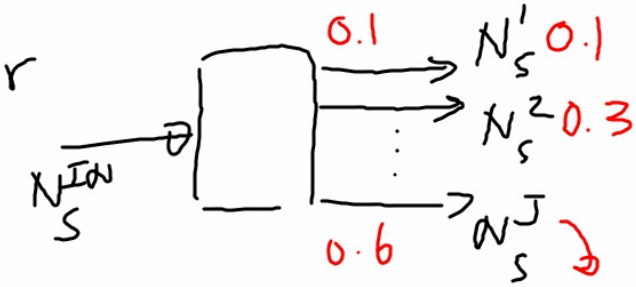
none

column
membrane
absorber/stripper



P4

## Flow splitter

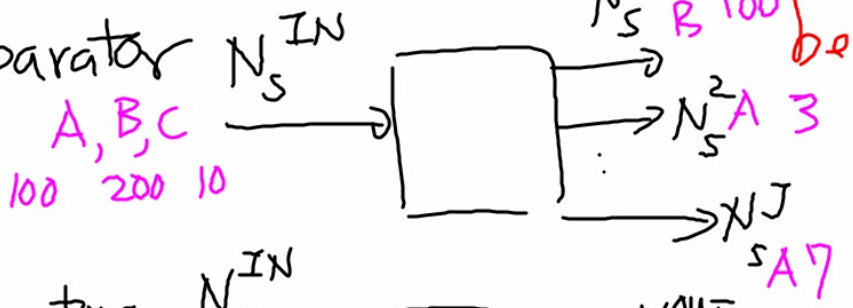



$$N_s^j = t^j N_s^{IN} \qquad j = 1, \ldots, J \qquad s = 1, \ldots, N$$

$1 - 0.1 - 0.3 = 0.6$ | split fraction going to stream $j$

because $\sum t^j = 1$ * standard input *

## Separator




$$N_s^j = t_s^j N_s^{IN}$$

split fraction of component $s$ in output stream $j$

standard input

## Reactor


$A + B \rightarrow C$

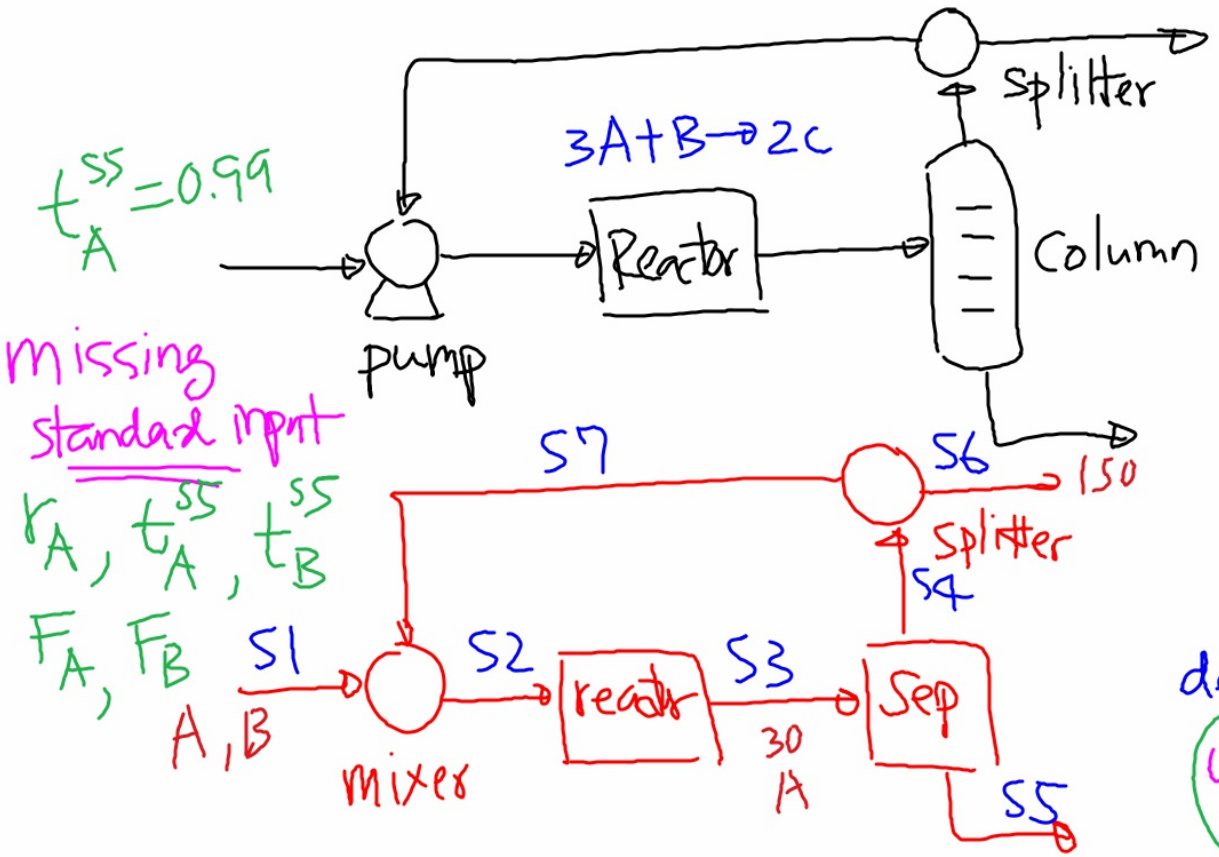
$3A + B \rightarrow 2C$

$3H_2 + N_2 \rightarrow 2NH_3$

stoichiometry | coefficients

fractional | conversion

P.5) # Example of a Flowsheet with Elementary Modules mass onl




$t_A^{S5} = 0.99$

missing standard input

$r_A$, $t_A^{S5}$, $t_B^{S5}$

$F_A$, $F_B$

Input Data: 4 targets

S 1. Split fraction to S6 = 40%

T 2. Total flow of S6 = 150 $\frac{lbmol}{hr}$

T 3. $X_B$ in S4 = 0.90

S 4. Mole-recovery of C in S5 = 95%

T 5. Reactor effluent contains $t_C^{S5}$ 30 lbmol/hr of A

T 6. S1 contains equimolar flow rates of A and B $\frac{F_A^{S1}}{F_B^{S1}} = 1.$

degree of freedom analysis!

(under-specified) over-specified fully-specified

p.6) Reactor:

$$N_s^{OUT} = N_s^{IN} + \sum_{i=1}^{R} \sigma_{s,i}\, r_i$$

- $\sigma_{s,i}$: stoic. coeff. — reactants, + products
- $r_i$: reactant
- $R$ = total # of rxns
- fractional conversion

(1) $A + B \rightarrow C$
(2) $A + D \rightarrow E$

} ~~parall~~ parallel rxns

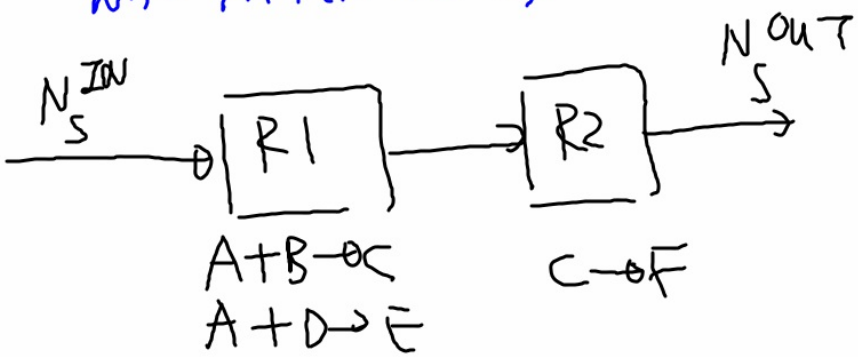
selectivity

overall $r_A = 0.9$ → $S_1 = 0.4$ $r_{A,1} = ?$ $(0.9)(0.4) = 0.36$

→ $S_2$ 0.6 $r_{A,2} = ?$ $(0.9)(0.6) = 0.54$ or $0.9 - 0.36 = 0.54$

(3) $C \rightarrow F$ (in series with Rxn (1) + (2))
$r_C = 0.5$

(4) $F \rightarrow G$




RSTOIC

fully-specified $\Rightarrow$ # of missing standard input $=$ # of design targets

under - $>$

over - $<$