CHEMICAL PROCESS CALCULATIONS

(Reactive process balance)

Lecture # 13: October 13, 2022

Reactive system balance

(a) molecular species balances (similar to nonreactive systems)

(b) atomic species balances

(c) extents of reaction

- independent equations
- independent species
- independent chemical reactions

Molecular species balances

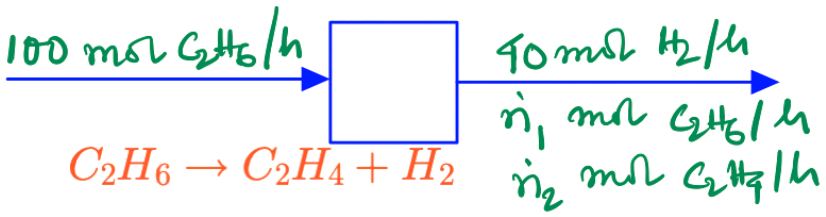
No. degrees of freedom =

No. unknown labeled variables

+ No. independent chemical reactions

- No. independent molecular species balances

- No. other equations relating unknown variables

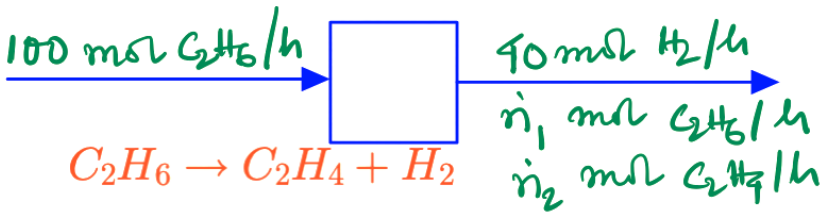


Atomic species balances

No. degrees of freedom =

No. unknown labeled variables

- No. independent atomic species balances
- No. molecular balances on independent nonreactive species
- No. other equations relating unknown variables



Balance using extent of reaction

No. degrees of freedom =

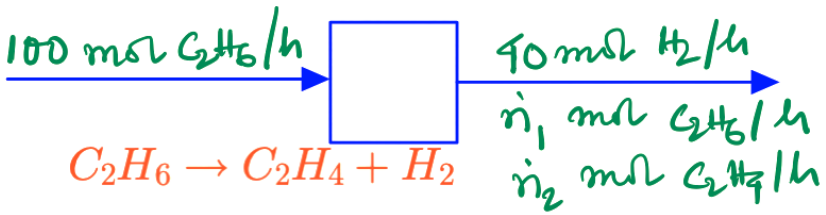
No. unknown labeled variables

+ No. independent reactions (one extent of reaction for each reaction)

- No. independent reactive species

- No. independent nonreactive species

- No. other equations relating unknown variables



Reactive system balance

- Atomic species balances:
  - straightforward solution procedure
  - less complicated for multiple reaction cases
- Extents of reaction:
  - convenient for chemical equilibrium problems
- Molecular species balances:
  - complex calculations
  - considered for simple systems (one reaction)

Methane is burned with air in a continuous steady-state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are:

$$CH_4 + 3/2\ O_2 = CO + 2H_2O$$

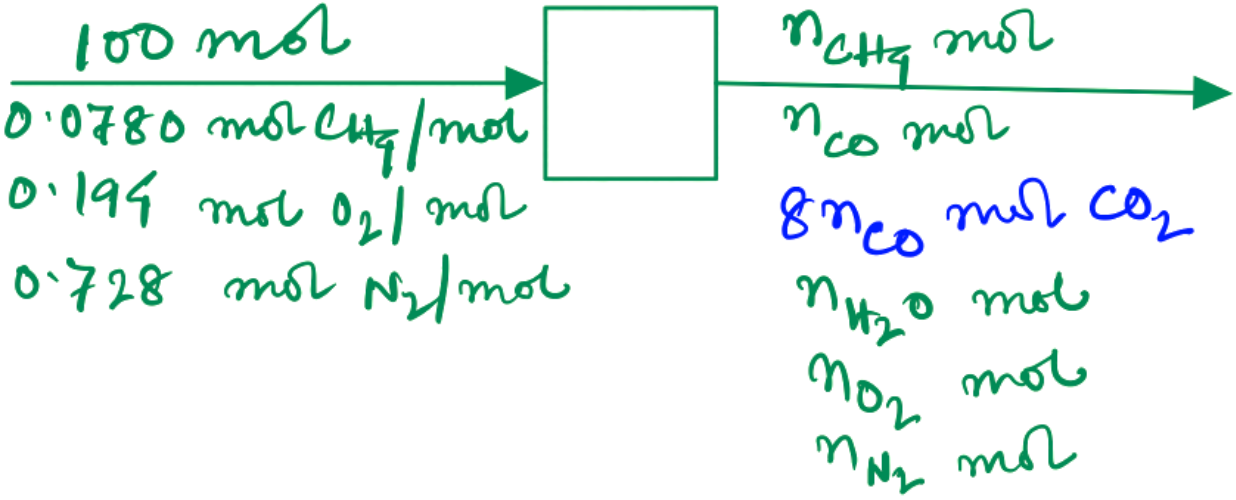
$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

The feed to the reactor contains 7.80 mole% CH_4 , 19.4% O_2 , and 72.8% N_2. The percentage conversion of methane is 90.0%, and the gas leaving the reactor contains 8 mol CO_2 /mol CO.

- Perform degree-of-freedom analysis on the process.
- Calculate the molar composition of the product stream using molecular species balances, atomic species balances, and extents of reaction.

$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$



MSB

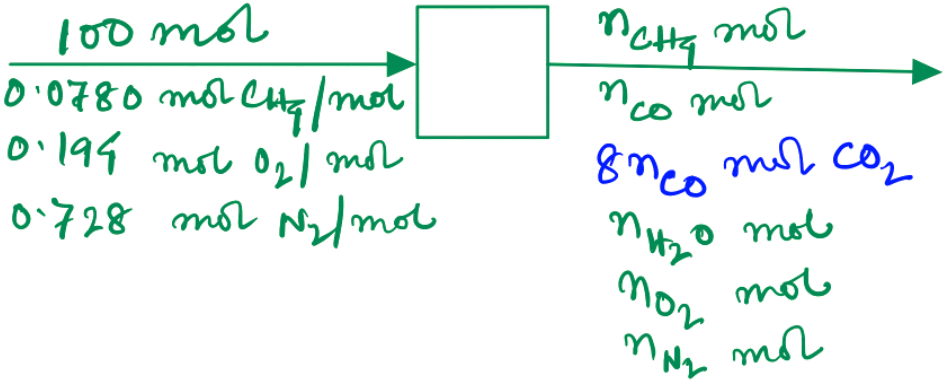
Unknown variables (5)

+ Independent reactions (2)

− n molecular species (6)

− Additional information (1)
(CH4 conversion)

DOF = 0



ASB

Unknown variables (5)
- Independent atomic species (3)
- Nonreactive molecular species (1)
- Additional information (1)
  (CH_4 conversion)

DOF = 0

EoR

Unknown variables (5)
+ Independent reactions (2)
- EoR expression for species (5)
- Nonreactive molecular species (1)
- Additional information (1)

DOF = 0