Process Simulation with ASPEN Plus

7505 Course Notes

Section 2: Mass-Balance Only Using

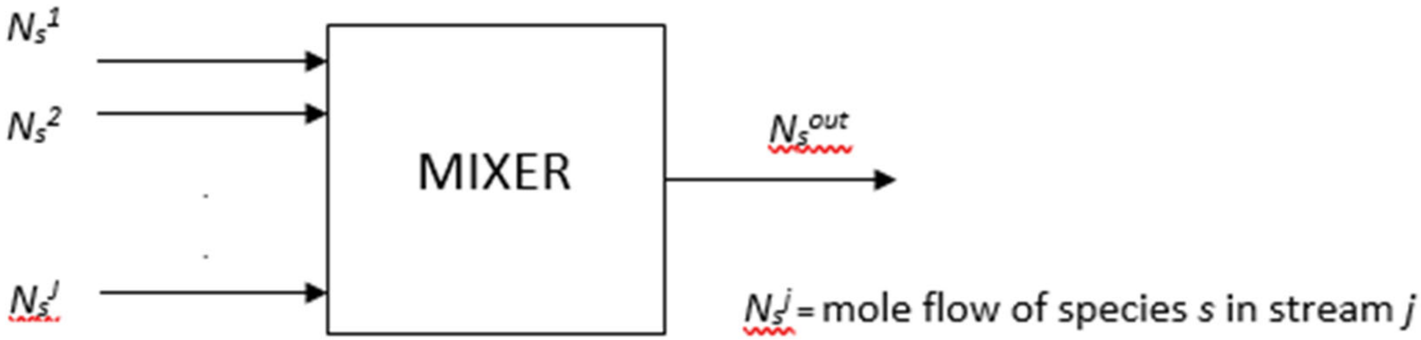
Elementary Modules with Standard Input

These course materials are applicable to Version 14 of ASPEN Plus

Mass-Balance Only in ASPEN Plus

- Mass-balance only is ONLY possible if "Elementary Modules" or models are used.
- There are 4 types of elementary modules which can represent practically every piece of equipment in a chemical process.
  1. Mixer (MIXER)
  2. Flow Splitter (FSPLIT)
  3. Component Separator (SEP)
  4. Reactor (RSTOIC)
- Each elementary module has its own standard input

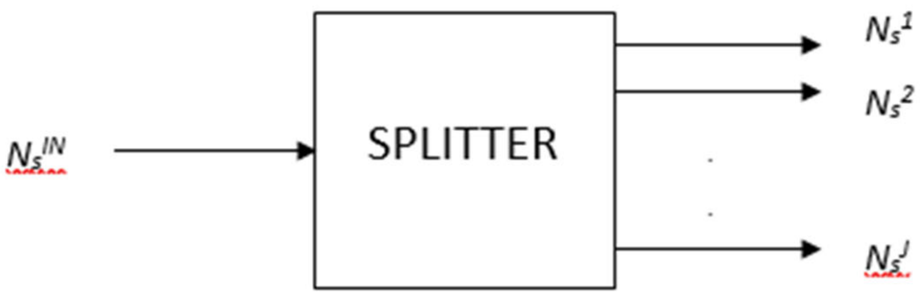
Elementary Module – The Mixer



$$N_S^{out} = \sum_{j=1}^{J} N_s^j \qquad s = 1, N$$

Standard specification: None, full information about the input

Elementary Module – The Flow Splitter



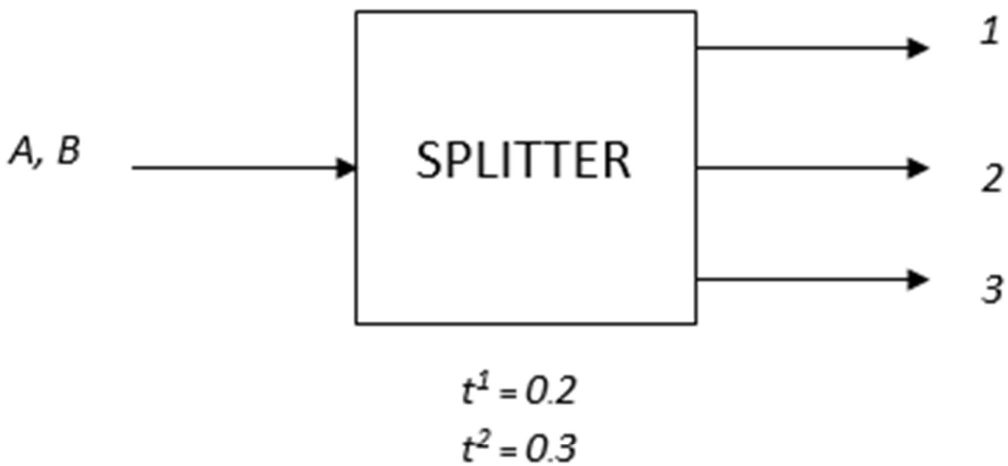
N_s^j = mole flow of species *s* in stream *j*

$$N_S^j = t^j N_s^{IN} \quad \forall \quad s = 1, N$$

Standard specification: split fraction t^j, $j = 1, 2, \ldots, J\text{-}1$

Notice that we always leave one stream unspecified because $\sum_{j=1}^{J} t^j = 1$

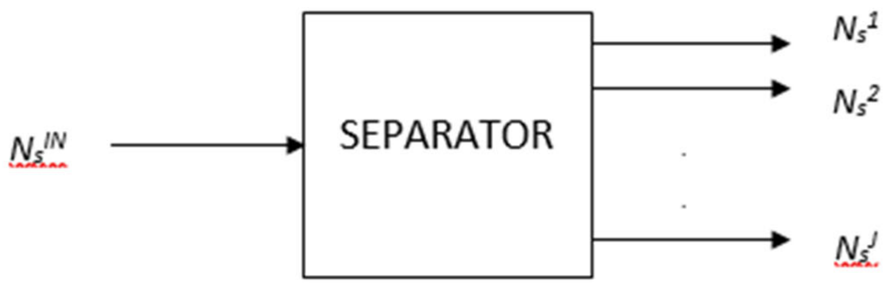
The Flow Splitter – Example



$$N_A^1 = 0.2 N_A^{IN} \qquad N_A^2 = 0.3 N_A^{IN}$$

$$N_B^1 = 0.2 N_B^{IN} \qquad N_B^2 = 0.3 N_B^{IN}$$

Elementary Module – The Component Separator



N_s^j = mole flow of species *s* in stream *j*

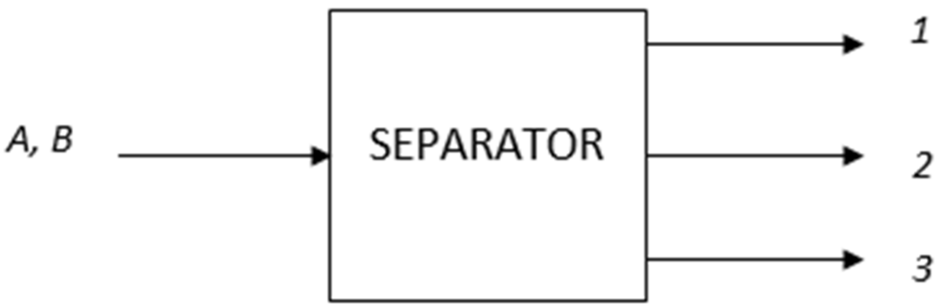
$$N_s^j = t_s^j + N_s^{IN} \quad \forall\ j = 1, 2, \dots, J, s = 1, 2, \dots, N$$

Standard specification: split fraction $t_s^j, j = 1, 2, \dots, J\text{-}1$ for all $s = 1, N$

$$\sum_{j=1}^{J} t_s^j = 1$$

Leave one stream unspecified too

The Component Separator – Example

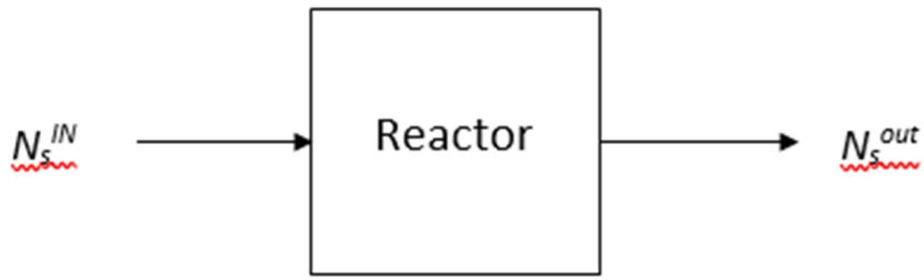


$$\left.\begin{array}{ll} t_A^1 = 0.8 & t_B^1 = 0.6 \\ t_A^2 = 0.1 & t_B^2 = 0.3 \end{array}\right\}\ \text{standard specifications}$$

$$t_A^3 = 0.1 \quad t_B^3 = 0.1$$

left unspecified

Elementary Module – The Reactor



$$N_S^{OUT} = N_s^{IN} + \left(\sum_{i=1}^{R} \sigma_{s,i}\ x_i\right) N_S^{IN}$$

where $\sigma_{s,i}$ = stoichiometric coefficient of species s in reaction i

x_i = fractional conversion of reaction i based on a key component

R = the total number of reactions

Assumption: All reactions take place *simultaneously* (or in parallel).

The Reactor – Example (Parallel Reactions)

<u>Parallel Reactions</u>:

$$A + B \rightarrow C \qquad 1^{st}\text{reaction conversion} = ?$$

$$A \rightarrow D + E \qquad 2^{nd}\text{reaction conversion} = ?$$

Overall conversion based on A is 80% with a selectivity of 60% for Reaction 1.

1st reaction conversion = $0.80 \times 0.60 = 0.48$

2nd reaction conversion = $0.80 \times 0.40 = 0.32$

0.80 which is the total conversion

$$N_A^{OUT} = N_A^{IN} - (0.48 + 0.32)N_A^{IN} \qquad N_D^{OUT} = N_D^{IN} + 0.32N_A^{IN}$$

$$N_B^{OUT} = N_B^{IN} - 0.48N_B^{IN} \qquad N_E^{OUT} = N_E^{IN} + 0.32N_E^{IN}$$

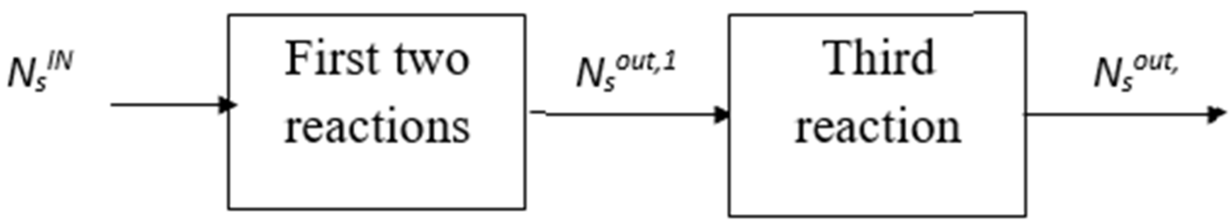
$$N_C^{OUT} = N_C^{IN} + 0.48N_C^{IN}$$

The Reactor – Example (Parallel + Serial Reactions)

Reactions in series:

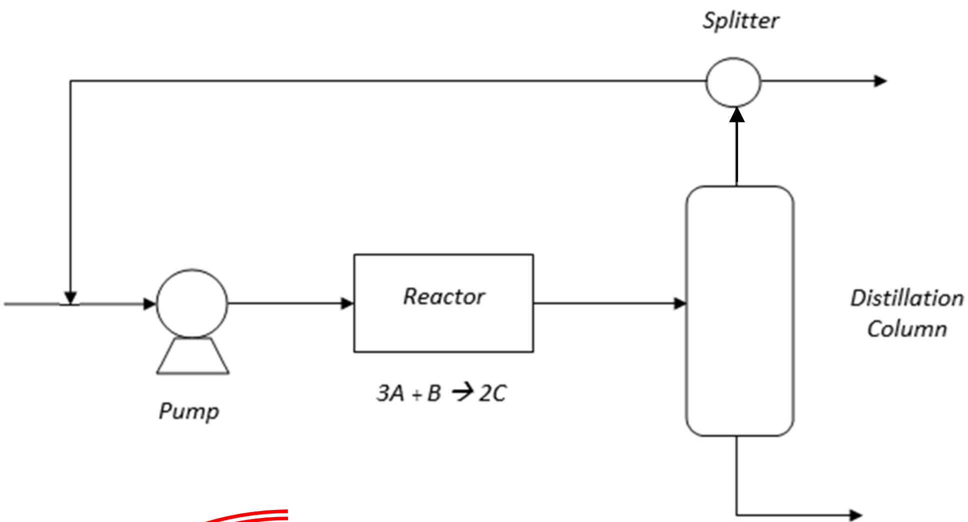
$$\left.\begin{array}{l} A+B \rightarrow C \\ \\ A \rightarrow D+E \end{array}\right\} \text{ Parallel reactions}$$

$$C \rightarrow F+G \qquad 3rd \;\; reaction \;\; conversion = 75\%$$

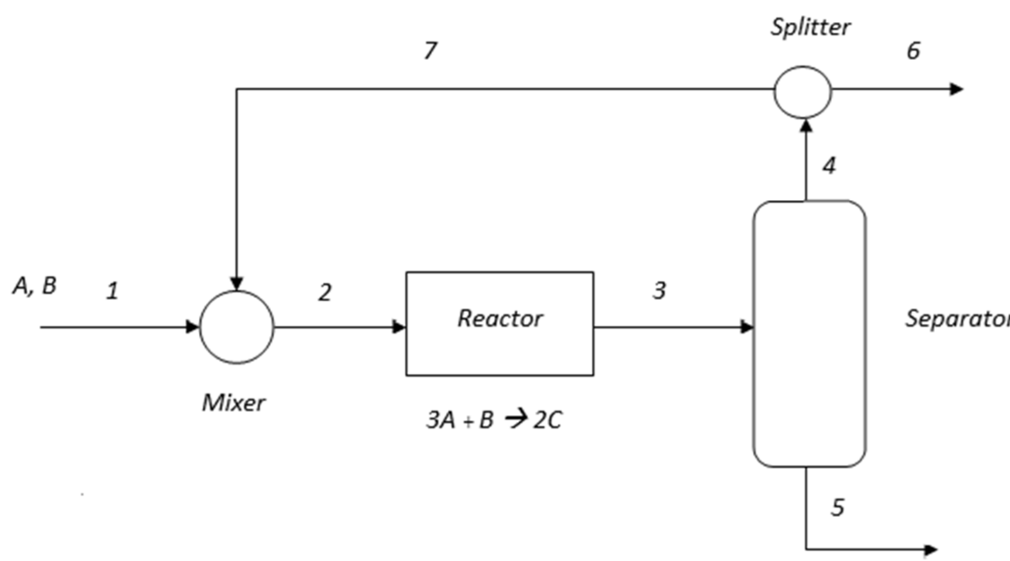


$$N_C^{OUT} = N_C^{OUT,1} - 0.75 N_C^{OUT,1} \quad and \quad N_C^{OUT,1} = N_C^{IN} + 0.48 N_A^{IN}$$

Example of a Process with Elementary Modules



Transformed into elementary modules



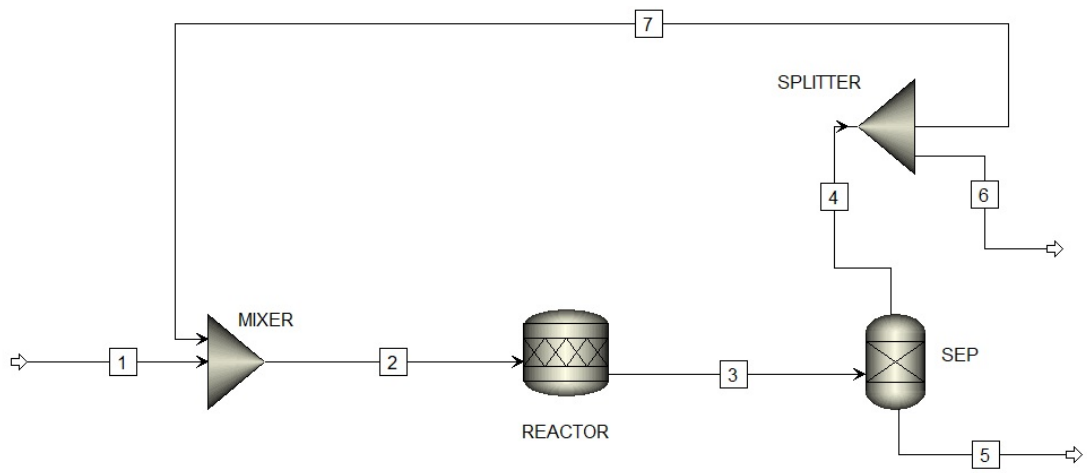
Elementary Modules in ASPEN Plus

- The Mixer = MIXER

- The Flow Splitter = FSPLIT

- The Component Separator = SEP

- The Mass-Balance Reactor = RSTOIC

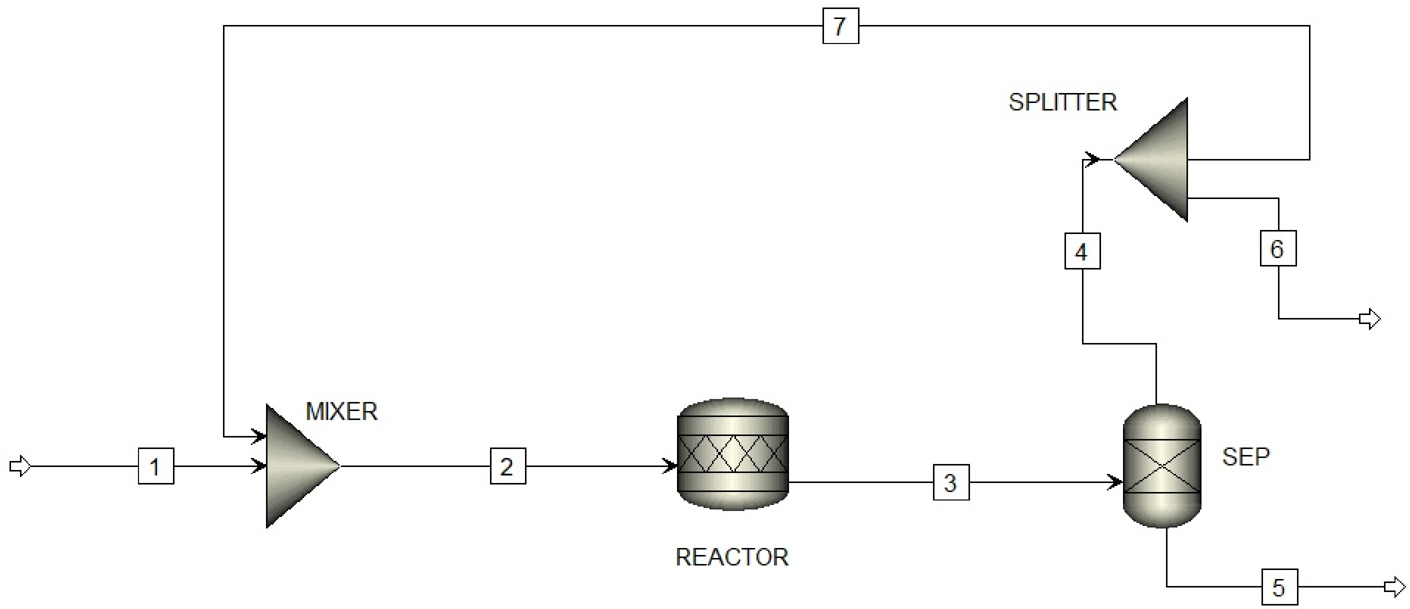


- Model/Module Name vs. Block ID

RSTOIC is the model name in ASPEN Plus which cannot be changed.

REACTOR is a Block ID specified by the user and can be changed to anything.

A+ Example of a Process with Elementary Modules



Our task: Perform a mass balance calculation of this process in A+ using standard input given for each elementary module.

First, learn to turn off energy balance by visiting Simulation → Setup → Calculation Options → Calculation and uncheck "Perform heat balance calculations"

Minimum Required Input Data for an A+ Model

Second, we must know the minimum required input data for a basic A+ model:

1. Process flowsheet, i.e. connectivity of all unit operation modules

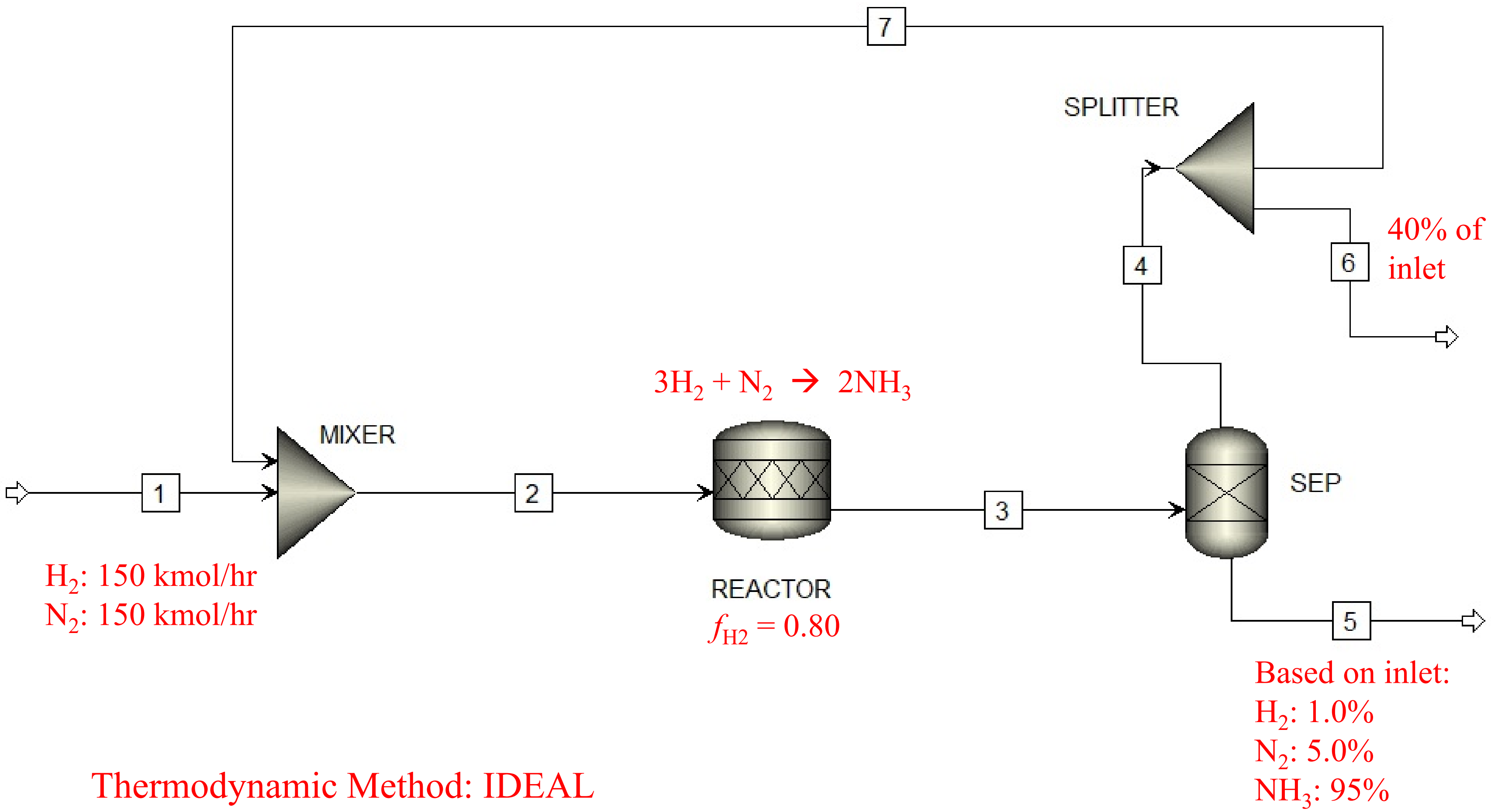
2. All chemical species (chemical components) present in the model

3. Process feed data: Total flow rate(s) and its/their composition(s) or individual component flow rates

4. Operating conditions of all unit operation modules

5. Thermodynamic package/method, e.g. ideal-gas/ideal-liquid, equations of state, etc. (can enter a dummy method if energy balance is turned off)

A+ Example with Elementary Modules (Cont'd)



Thermodynamic Method: IDEAL
(dummy, because we are not doing energy balance)

Introduction to ASPEN PLUS User Interface

- GUI consists of 2 main components

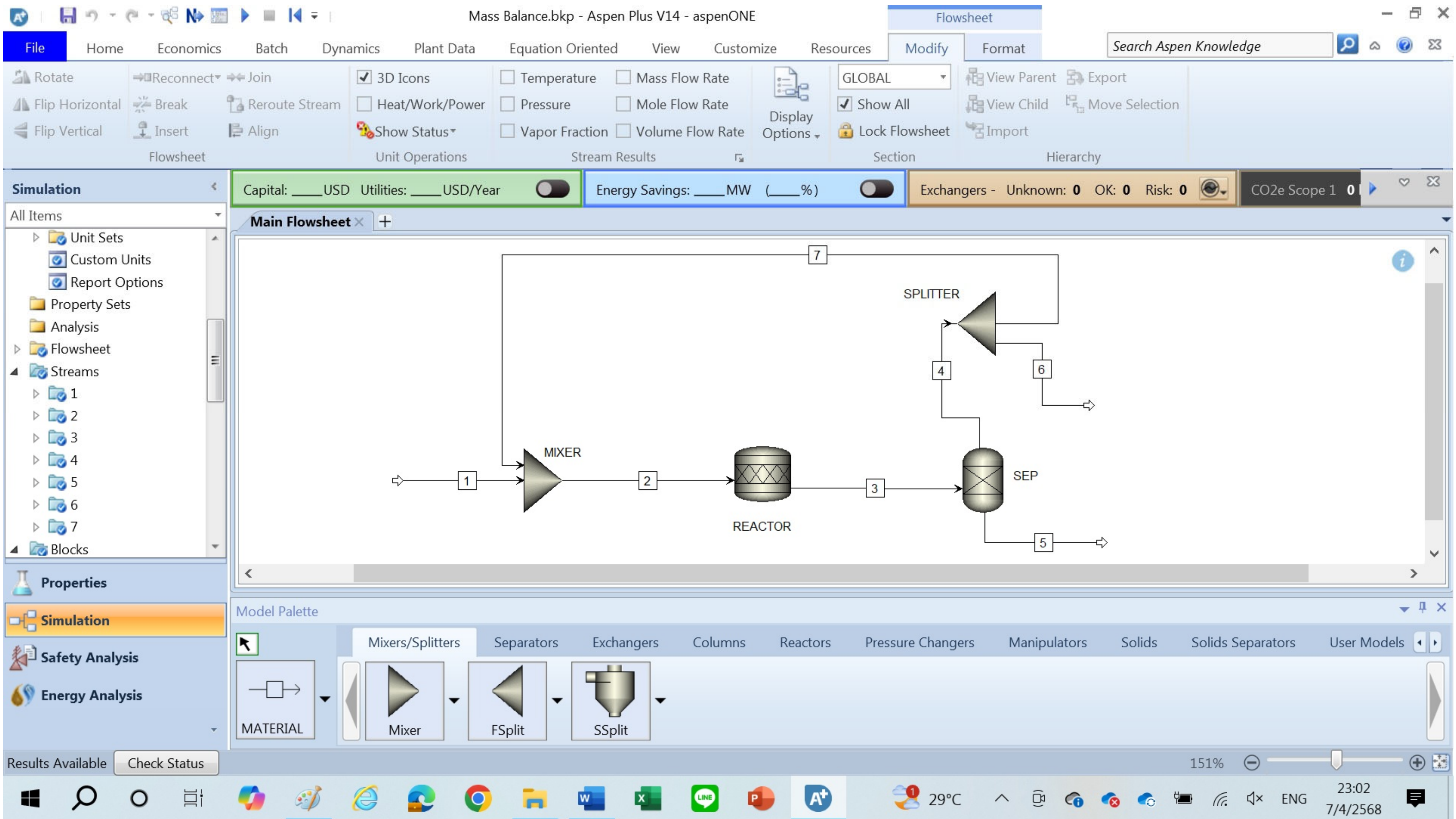
  1. Graphics

     - Flowsheet graphics
     - Results plots
     - Process flow diagrams (PFD) generation

  2. Forms and Menus

     - Help you enter process data, such as components, properties, unit operations, and other specifications to define your problem

Mass-Balance Only: A+ Model



Mass-Balance Only: Stream Summary/Table