

# Process Simulation with ASPEN Plus

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## 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

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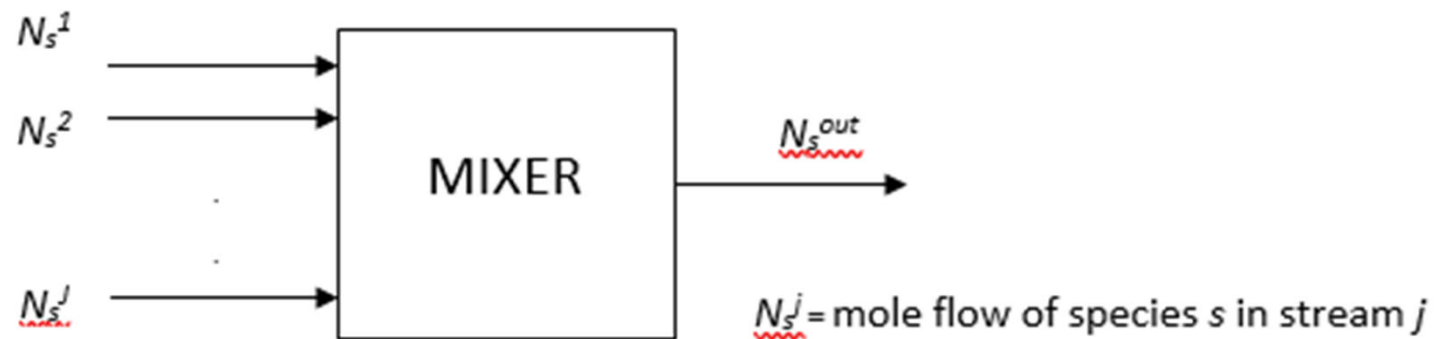
# Mass-Balance Only in ASPEN Plus

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- ❑ 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

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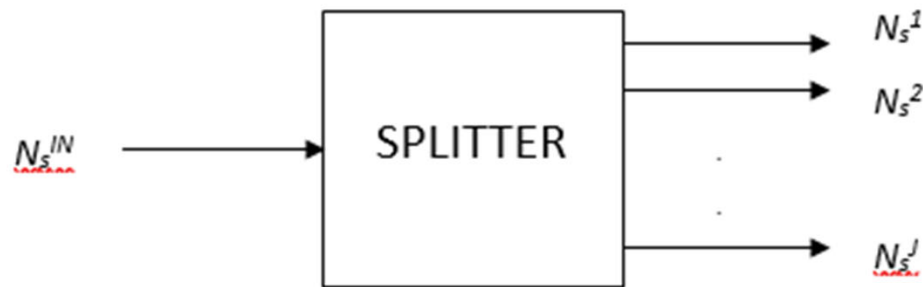


$$N_s^{out} = \sum_{j=1}^J N_s^j \quad s = 1, N$$

Standard specification: None, full information about the input

# Elementary Module – The Flow Splitter

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

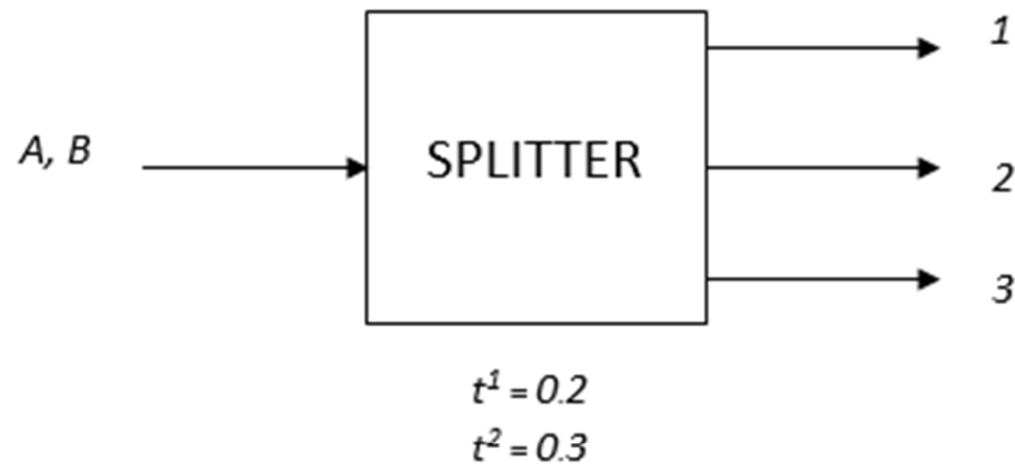
$$N_s^j = t^j N_s^{IN} \quad \forall \quad s = 1, N$$

Standard specification: split fraction  $t^j, j = 1, 2, \dots, J-1$

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

# The Flow Splitter – Example

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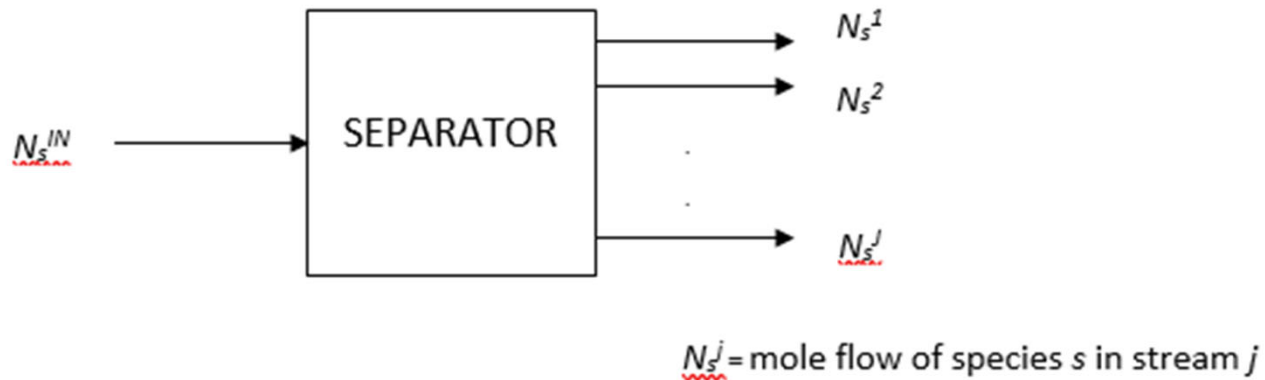


$$N_A^1 = 0.2 N_A^{IN} \quad N_A^2 = 0.3 N_A^{IN}$$

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

# Elementary Module – The Component Separator

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

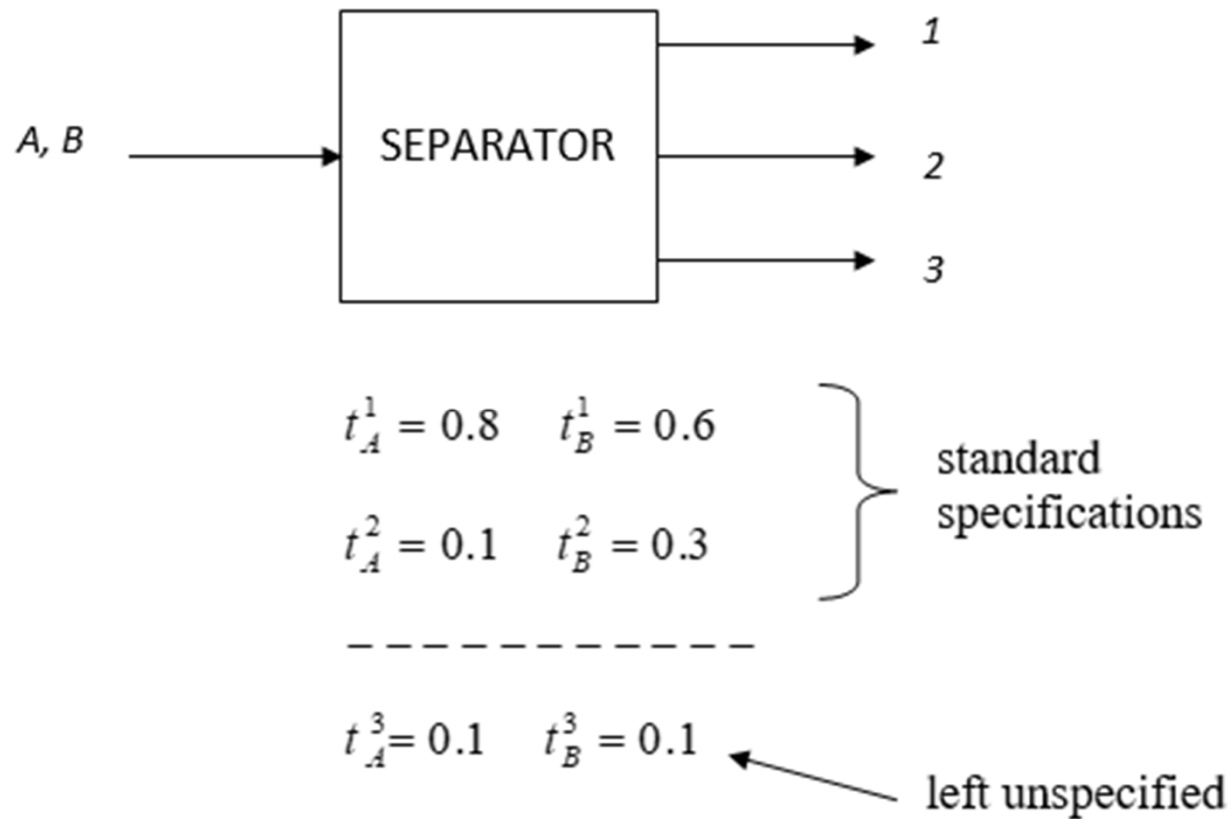
Standard specification: split fraction  $t_s^j, j = 1, 2, \dots, J-1$  for all  $s = 1, N$

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

Leave one stream unspecified too

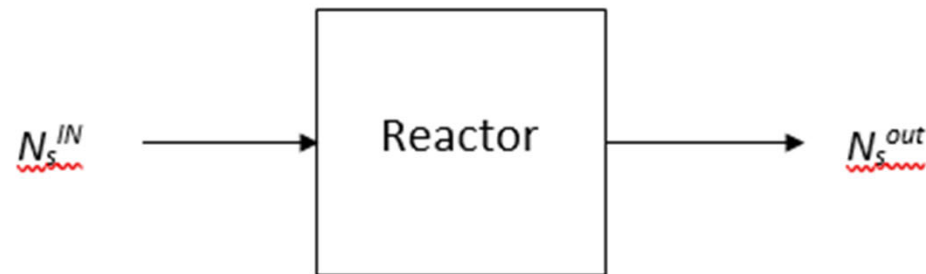
# The Component Separator – Example

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# Elementary Module – The Reactor

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

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)

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Parallel Reactions:



1<sup>st</sup> reaction conversion = ?



2<sup>nd</sup> reaction conversion = ?

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

$$1^{\text{st}} \text{ reaction conversion} = 0.80 \times 0.60 = 0.48$$

$$2^{\text{nd}} \text{ reaction conversion} = 0.80 \times 0.40 = 0.32$$

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0.80    which is the total conversion

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

$$N_D^{OUT} = N_D^{IN} + 0.32N_A^{IN}$$

$$N_B^{OUT} = N_B^{IN} - 0.48N_A^{IN}$$

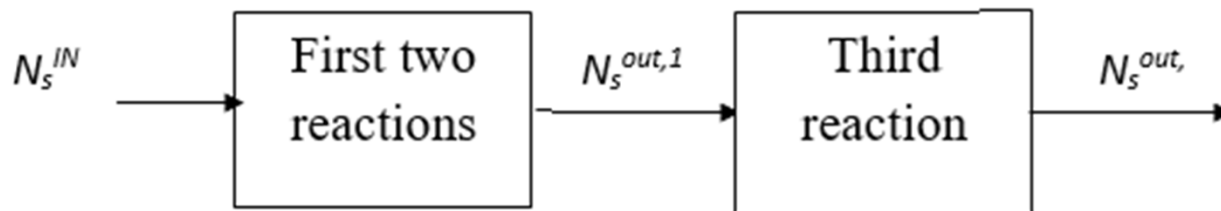
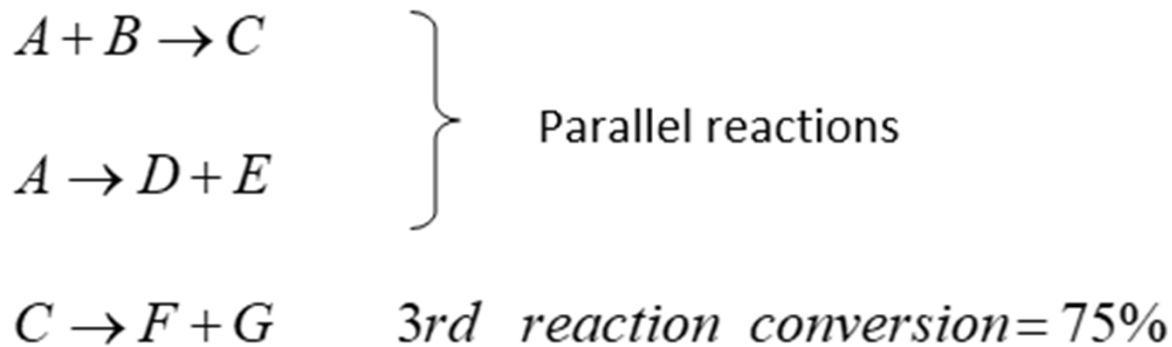
$$N_E^{OUT} = N_E^{IN} + 0.32N_A^{IN}$$

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

# The Reactor – Example (Parallel + Serial Reactions)

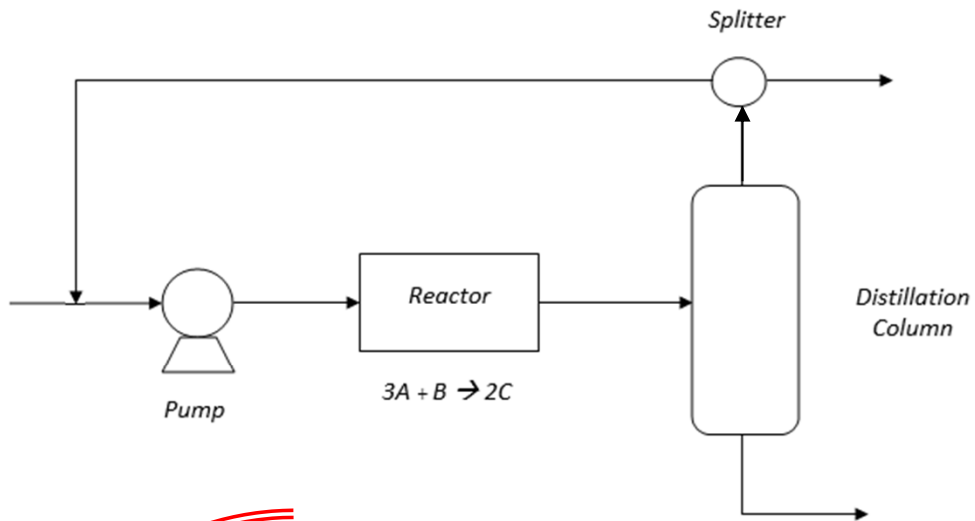
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Reactions in series:

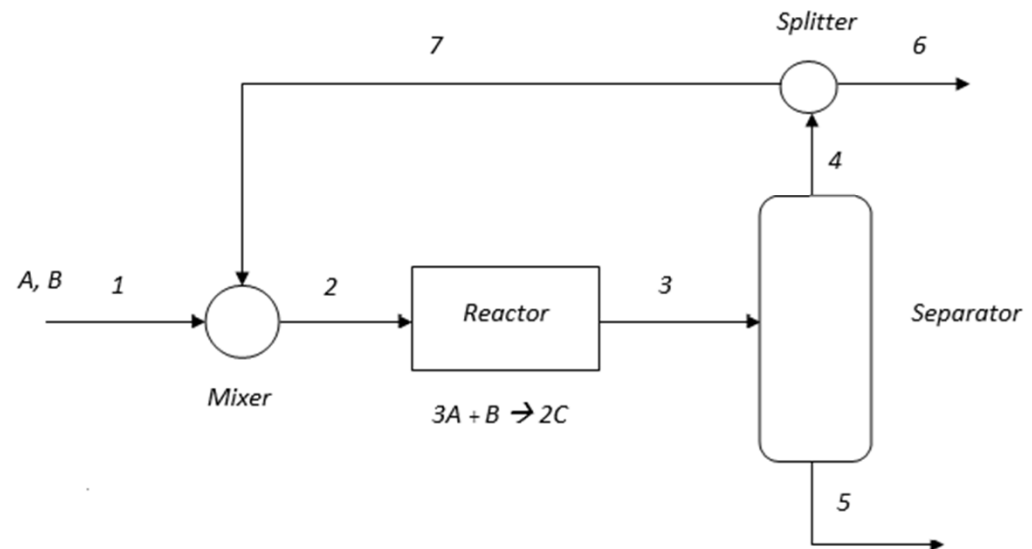


$$N_C^{OUT} = N_C^{OUT,1} - 0.75N_C^{OUT,1} \quad \text{and} \quad N_C^{OUT,1} = N_C^{IN} + 0.48N_A^{IN}$$

# Example of a Process with Elementary Modules



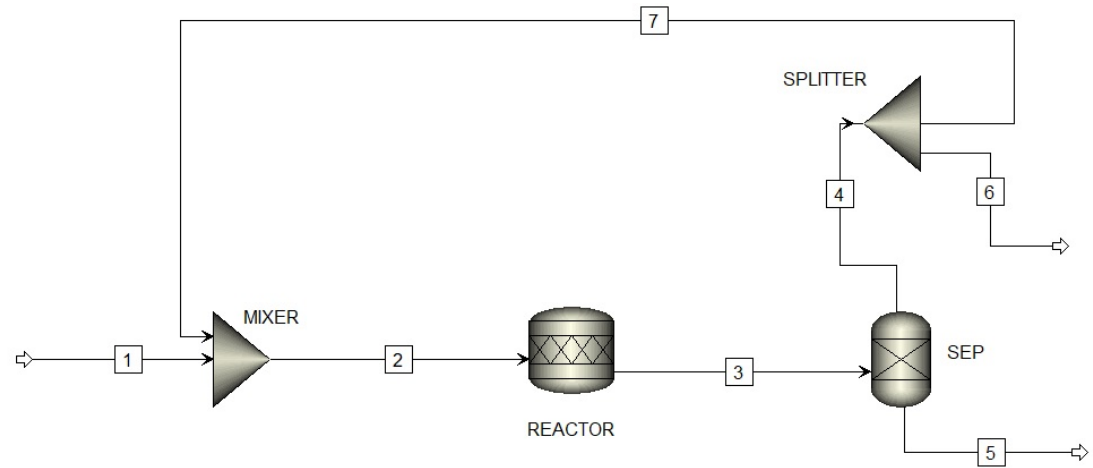
Transformed into  
elementary modules



# Elementary Modules in ASPEN Plus

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- ❑ The Mixer = **MIXER**
- ❑ The Flow Splitter = **FSPLIT**
- ❑ The Component Separator = **SEP**
- ❑ The Mass-Balance Reactor = **RSTOIC**
- ❑ Model/Module Name vs. Block ID

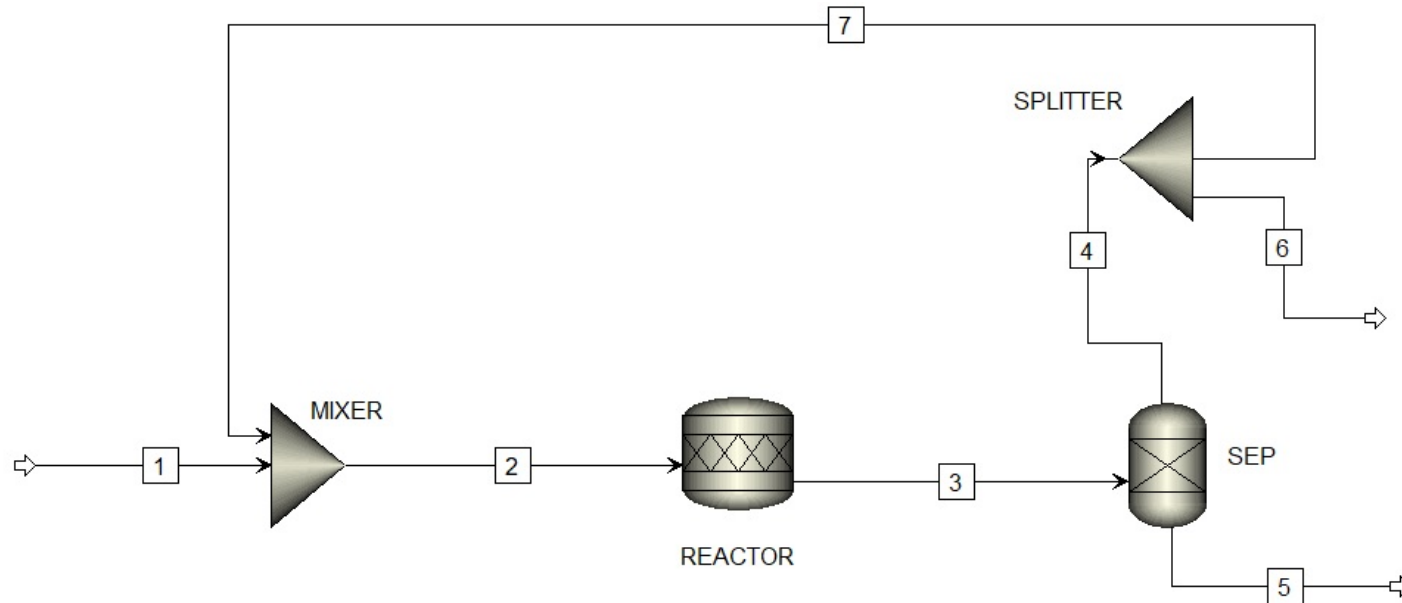


RSTOIC is the model name in ASPEN Plus which cannot be changed.

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

# A+ Example of a Process with Elementary Modules

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**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”

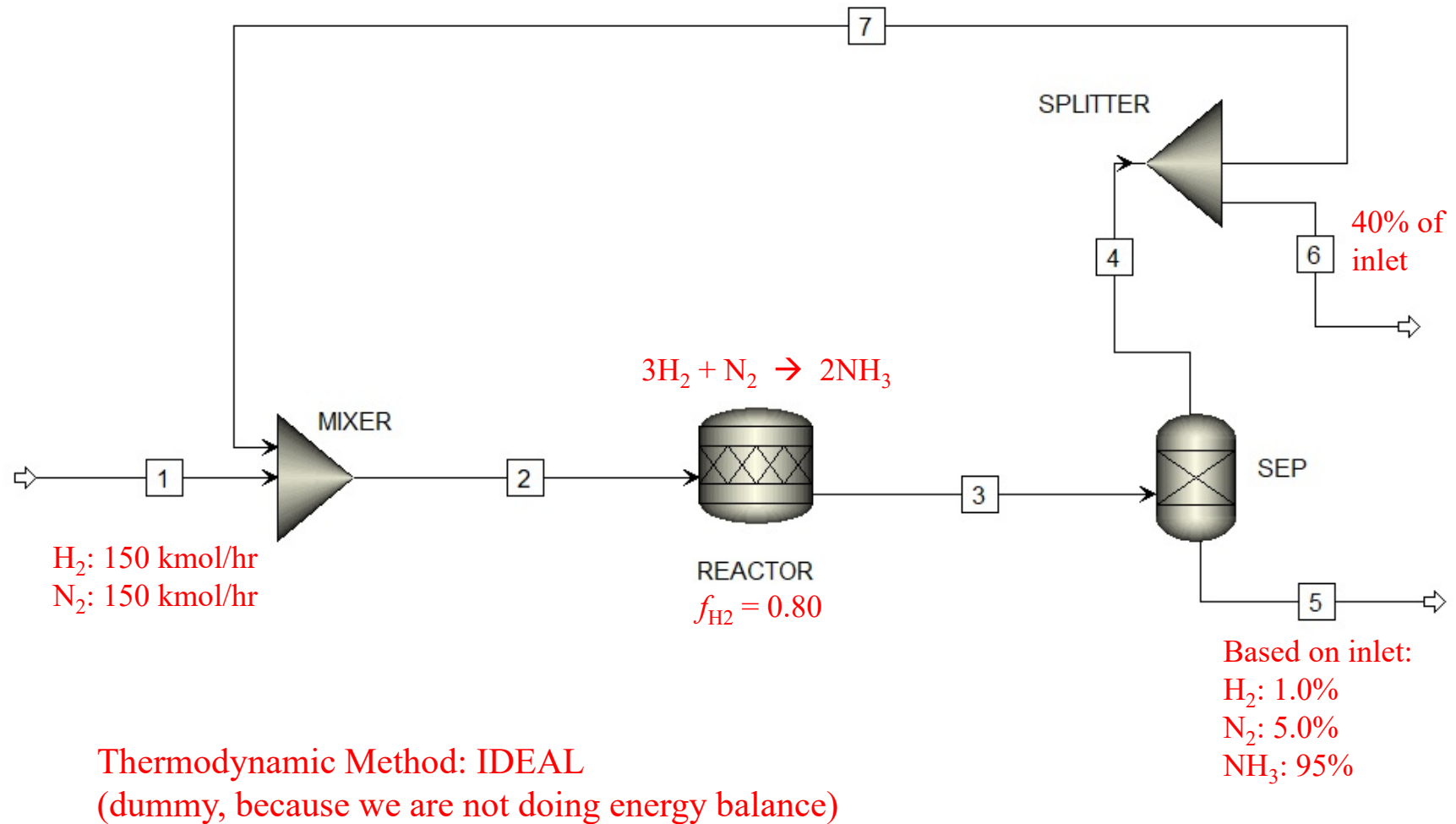
# Minimum Required Input Data for an A+ Model

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**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)



# Introduction to ASPEN PLUS User Interface

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□ GUI consists of 2 main components

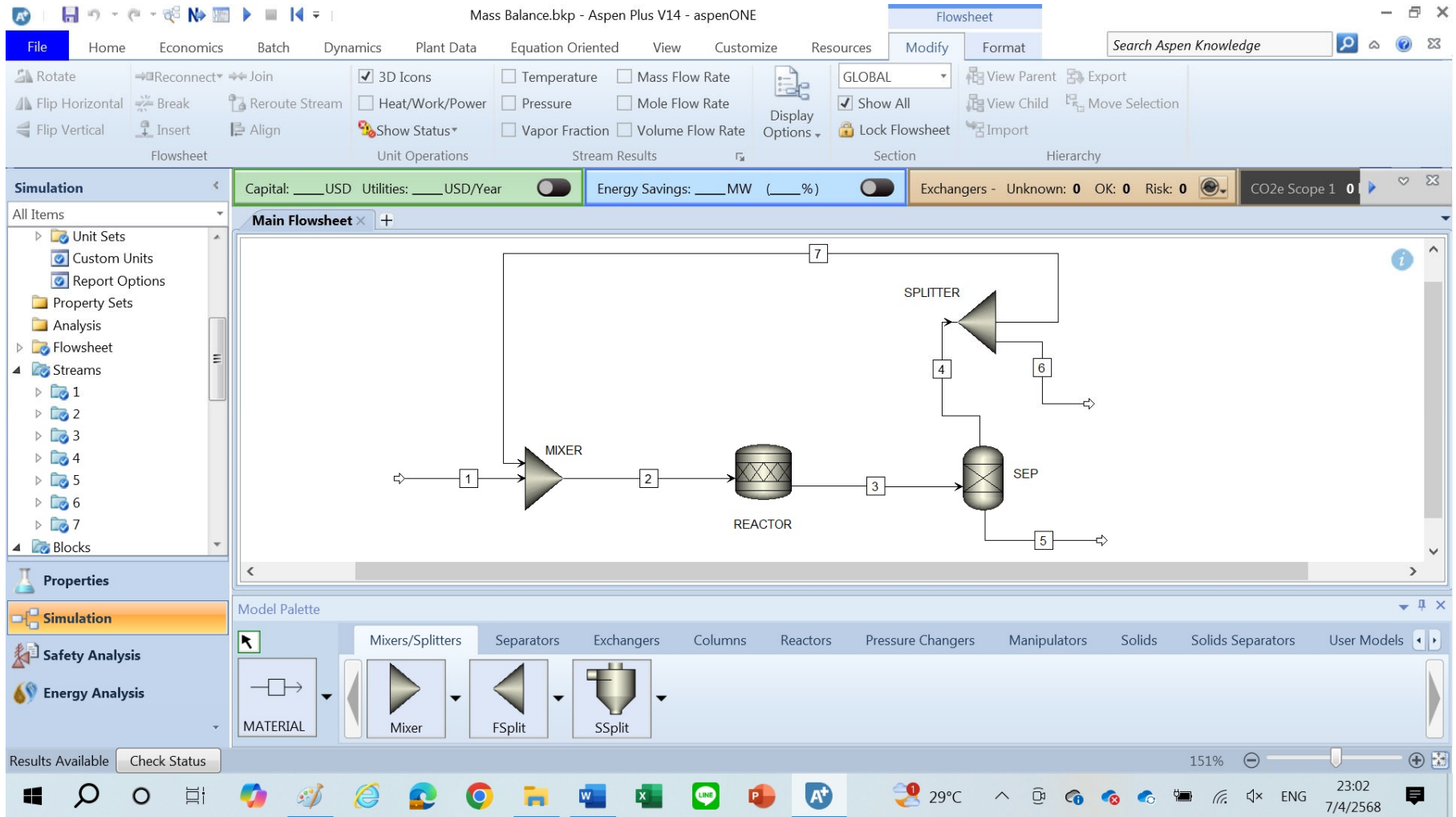
## 1. Graphics

- 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

Mass-Balance Only A+ Model - Minimum Required Input.bkp - Aspen Plus V14 - aspenONE

File Home Economics Batch Dynamics Plant Data Equation Oriented View Customize Resources Report

Stream Summary

Search Aspen Knowledge

Save Save as New Show Child Hierarchy Streams Stream Group

Full Save Save as New Discard Change Template

General Options

Stream Summary Options

Flows Composition

Property Sets

Report

Simulation

Capital: \_\_\_USD Utilities: \_\_\_USD/Year Energy Savings: \_\_\_MW (\_\_\_%) Exchangers - Unknown: 0 OK: 0 Risk: 0 CO2e Scope 1 0

Main Flowsheet Results Summary - Streams (All)

| Material                | Heat          | Load          | Work           | Power          | Vol.% Curves   | Wt.% Curves    | Petroleum      | Polymers       | Solids |
|-------------------------|---------------|---------------|----------------|----------------|----------------|----------------|----------------|----------------|--------|
| Enthalpy Flow           | cal/sec       | -2.9885e+34   |                |                |                |                |                |                |        |
| Average MW              |               | 15.0147       | 18.3616        | 22.8559        | 24.5714        | 18.2974        | 24.5714        | 24.5714        |        |
| <b>- Mole Flows</b>     | <b>kmo...</b> | <b>300</b>    | <b>461.696</b> | <b>370.91</b>  | <b>269.493</b> | <b>101.418</b> | <b>107.797</b> | <b>161.696</b> |        |
| H2                      | kmol...       | 150           | 170.222        | 34.0445        | 33.704         | 0.340445       | 13.4816        | 20.2224        |        |
| N2                      | kmol...       | 150           | 288.666        | 243.273        | 231.109        | 12.1636        | 92.4437        | 138.666        |        |
| NH3                     | kmol...       | 0             | 2.80779        | 93.5931        | 4.67965        | 88.9134        | 1.87186        | 2.80779        |        |
| <b>- Mole Fractions</b> |               |               |                |                |                |                |                |                |        |
| H2                      |               | 0.5           | 0.36869        | 0.0917863      | 0.125065       | 0.00335686     | 0.125065       | 0.125065       |        |
| N2                      |               | 0.5           | 0.625229       | 0.65588        | 0.857571       | 0.119936       | 0.857571       | 0.857571       |        |
| NH3                     |               | 0             | 0.00608148     | 0.252333       | 0.0173647      | 0.876707       | 0.0173647      | 0.0173647      |        |
| <b>- Mass Flows</b>     | <b>kg/hr</b>  | <b>4504.4</b> | <b>8477.49</b> | <b>8477.49</b> | <b>6621.82</b> | <b>1855.68</b> | <b>2648.73</b> | <b>3973.09</b> |        |
| H2                      | kg/hr         | 302.382       | 343.148        | 68.6296        | 67.9433        | 0.686296       | 27.1773        | 40.766         |        |
| N2                      | kg/hr         | 4202.02       | 8086.53        | 6814.92        | 6474.17        | 340.746        | 2589.67        | 3884.5         |        |
| NH3                     | kg/hr         | 0             | 47.8183        | 1593.94        | 79.6971        | 1514.25        | 31.8789        | 47.8183        |        |

Results Available Check Status

100%

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