

Introduction to Aspen Plus

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Date: 2013/09/02

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Introduction to Aspen Plus

Part 1: Introduction

What is Aspen Plus

- Aspen Plus is a market-leading process modeling tool for conceptual design, optimization, and performance monitoring for the chemical, polymer, specialty chemical, metals and minerals, and coal power industries.

What Aspen Plus provides

- **Physical Property Models**
 - World's largest database of pure component and phase equilibrium data for conventional chemicals, electrolytes, solids, and polymers
 - Regularly updated with data from U. S. National Institute of Standards and Technology (NIST)
- **Comprehensive Library of Unit Operation Models**
 - Addresses a wide range of solid, liquid, and gas processing equipment
 - Extends steady-state simulation to dynamic simulation for safety and controllability studies, sizing relief valves, and optimizing transition, startup, and shutdown policies
 - Enables you build your own libraries **using Aspen Custom Modeler or programming languages (User-defined models)**

More Detailed

- **Properties analysis**
 - Properties of pure component and mixtures (Enthalpy, density, viscosity, heat capacity,...etc)
 - Phase equilibrium (VLE, VLLE, azeotrope calculation...etc)
 - Parameters estimation for properties models (UNIFAC method for binary parameters, Joback method for boiling points...etc)
 - Data regression from experimental data
- **Process simulation**
 - pump, compressor, valve, tank, heat exchanger, CSTR, PFR, distillation column, extraction column, absorber, filter, crystallizer...etc

What course Aspen Plus can be employed for

- MASS AND ENERGY BALANCES
- PHYSICAL CHEMISTRY
- CHEMICAL ENGINEERING THERMODYNAMICS
- CHEMICAL REACTION ENGINEERING
- UNIT OPERATIONS
- PROCESS DESIGN
- PROCESS CONTROL

Lesson Objectives

- Familiar with the interface of Aspen Plus
- Learn how to use properties analysis
- Learn how to setup a basic process simulation

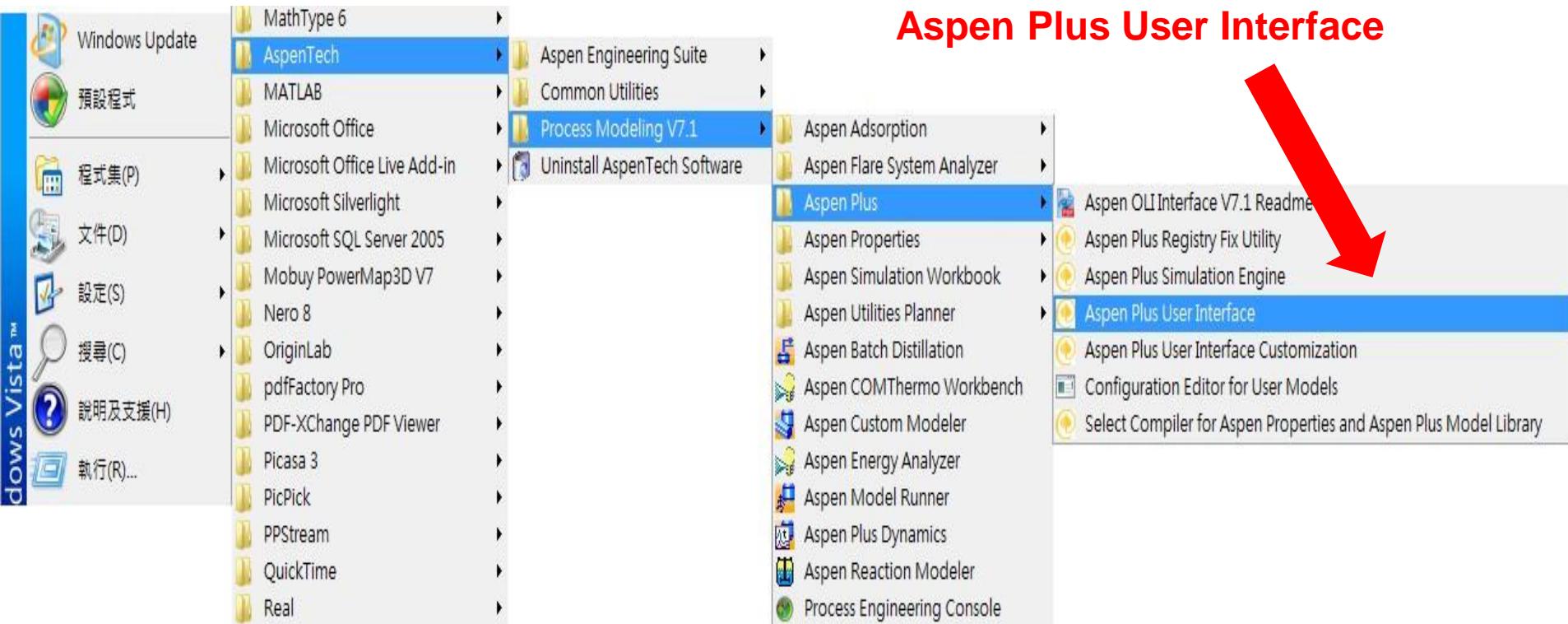
Outline

- Part 1 : Introduction
- Part 2 : Startup
- Part 3 : Properties analysis
- Part 4 : Running Simulation in Aspen Plus (simple units)
- Part 5 : Running Simulation in Aspen Plus (Reactors)
- Part 6 : Running Simulation in Aspen Plus (Distillation)
- Part 7 (additional): Running Simulation in Aspen Plus (Design, spec and vary)

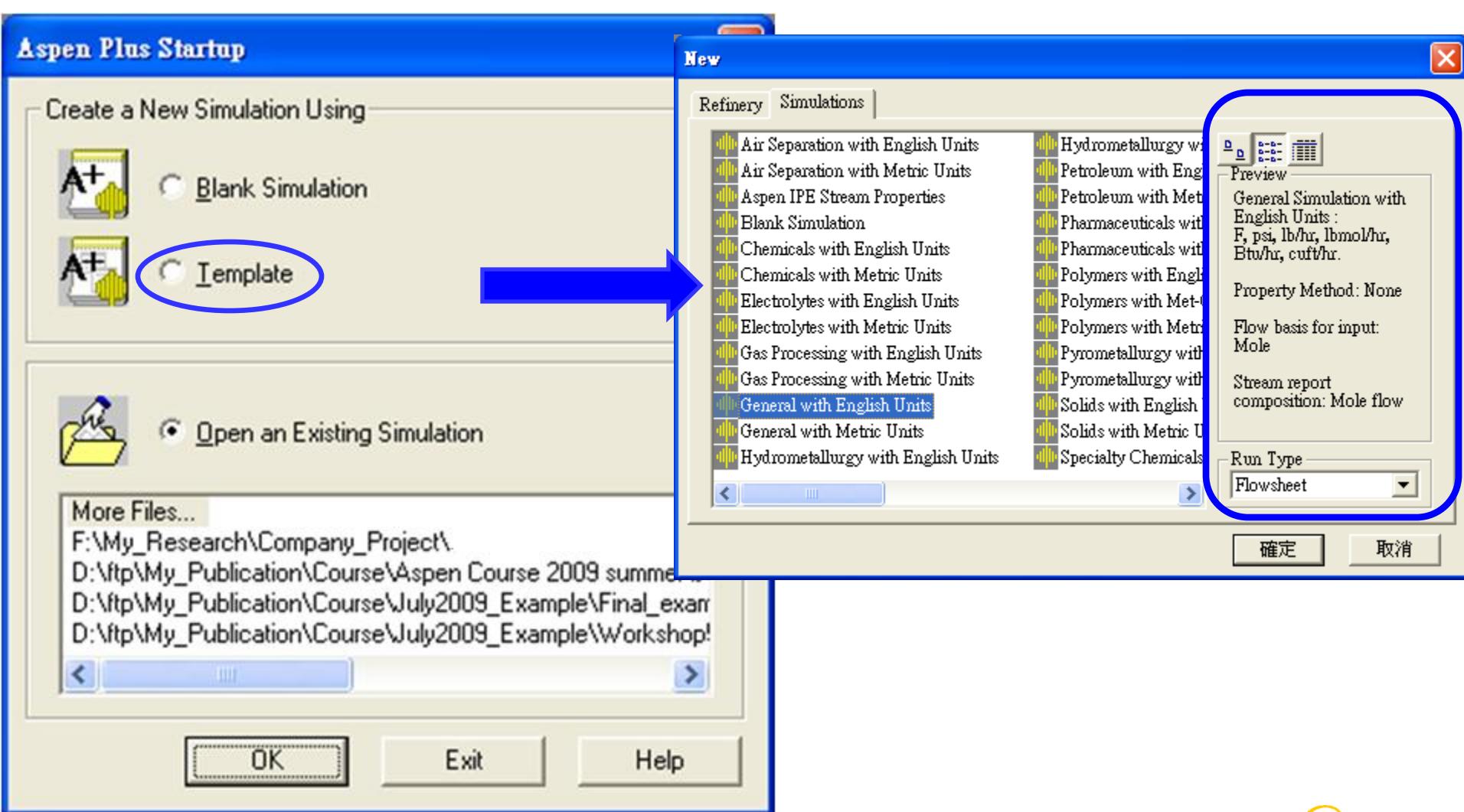
Introduction to Aspen Plus

Part 2: Startup

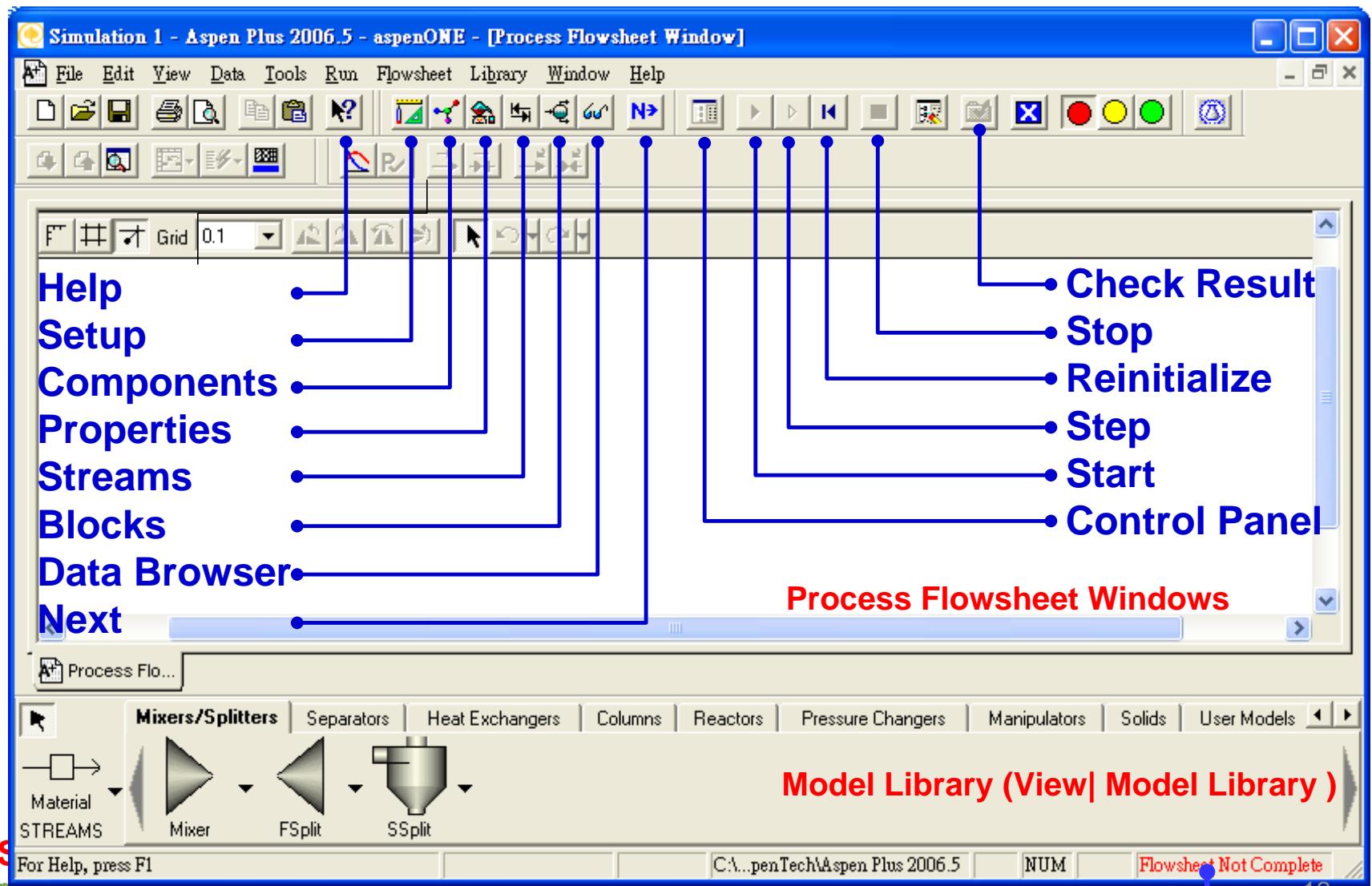
Start with Aspen Plus



Aspen Plus Startup



Interface of Aspen Plus



More Information

Aspen Plus Help

隱藏頁籤 上一頁 下一頁 首頁 列印 選項(O)

內容(C) 索引(N) 搜尋(S)

鍵入所要尋找的關鍵字(W): Commands for Controlling Simulations

列出主題(L)

選取所要顯示的主題(I):

- Changing Run Settings and User Databanks
- Command Line Options
- Commands for Controlling Simulations
- Displaying Forms and Sheets in the Data Br...
- EO Configuration for Compressor Kickback
- EO Configuration for Feed Tray Optimization
- EO Configuration for Tiered Pricing
- File Formats in Aspen Plus
- Information Transfer to Aspen Process Eco...
- Run Move To
- Run Stop Points
- Running the EO Strategy
- Running the Simulation Interactively
- Soft Bounds
- Unit Operation Summary
- Viewing LSSQP Iteration Summary Informati...
- Viewing Simulation Status Using the Control...

Commands for Controlling Simulations

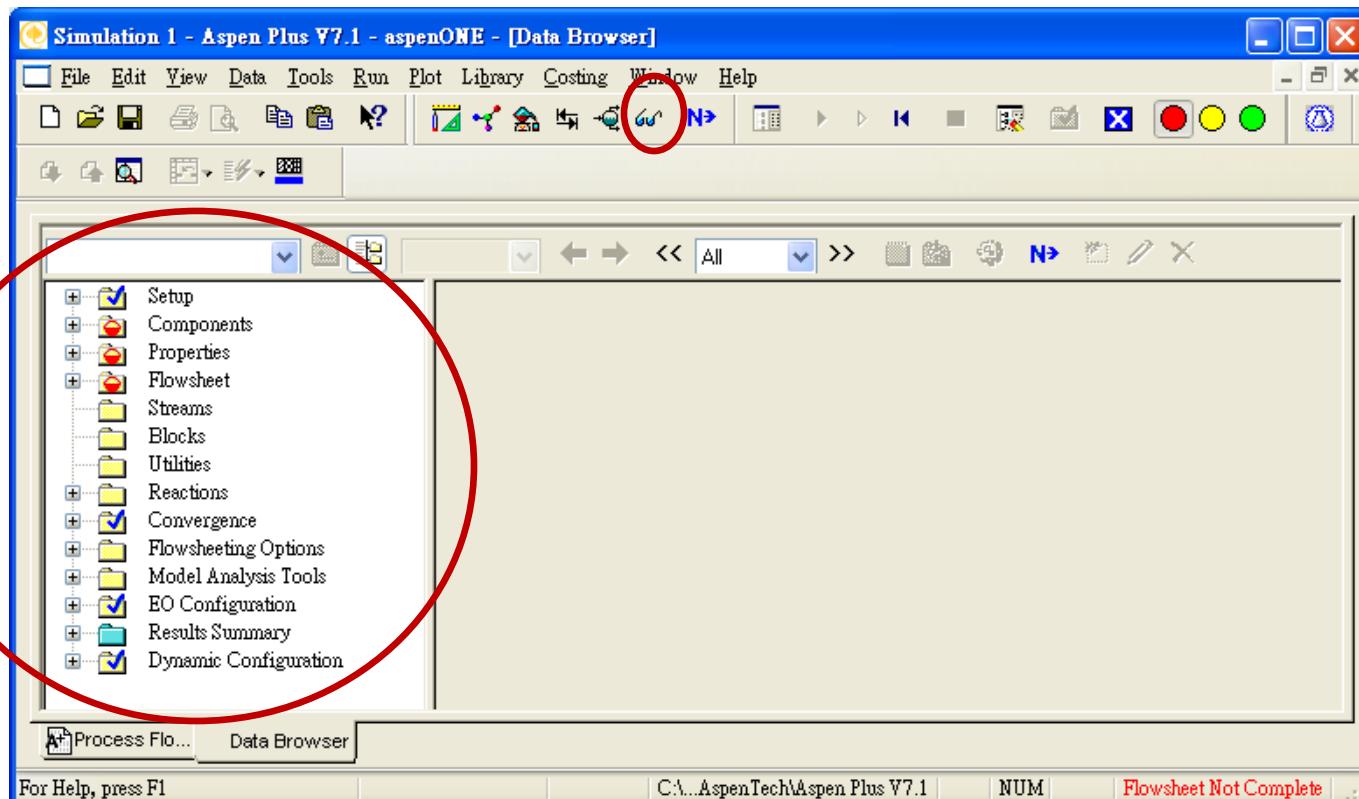
You can control the simulation by using the commands on the Run menu, the Simulation Run toolbar, or the Control Panel:

To	Do this
Start or continue calculations (Complete and On Demand run modes)	Click the Start button  on the toolbar.
Pause simulation calculations	Click the Stop button  on the toolbar.
Step through the flowsheet one block at a time	Click the SM Step button  on the toolbar. You can use the SM Step button to step through an SM simulation to the point where you wish to change to EO mode. The SM Step button is unavailable in EO mode because there are no sequential steps in an EO operation. For EO mode, the SM Step button can be used to select an initialization point in SM mode before switching to EO mode.
Control how far the SM simulation is converged	Select <i>Solve</i> from the SM Solution Strategy field  <i>Solve</i>  on the toolbar to fully solve the simulation in an SM run. Select <i>Single Pass</i> to execute each block once only in an SM run each time you click the start button. Select <i>Single Pass: Changed</i> to execute only new

Help for Commands for Controlling Simulations

Data Browser

- The Data Browser is a sheet and form viewer with a hierarchical tree view of the available simulation input, results, and objects that have been defined



Setup – Specification

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Setup Specifications - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Costir

Specifications

Setup

- ✓ Specifications
- ✓ Simulation Options
- ✓ Stream Class
- + Substreams
- + Costing Options
- + Stream Price
- + Units-Sets
- + Custom Units
- + Report Options

Components

Properties

+ Flowsheet

- Streams
- Blocks
- Utilities
- Reactions
- Convergence
- Flowsheeting Options
- Model Analysis Tools
- + EO Configuration
- + Results Summary
- + Dynamic Configuration

Process Flo... Setup Specif...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User M

Material STREAMS Mixer FSplit SSplit

C:\AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

Global Description Accounting Diagnostics

Title: [REDACTED]

Units of measurement: Input data: METCBA Output results: METCBA

Global settings:

- Run type: Flowsheet
- Input mode: Steady-State
- Stream class: CONVEN
- Flow basis: Mole
- Ambient pressure: 1.01325 bar
- Ambient temp.: 10 °C
- Valid phases:
- Free water: No

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Run Type

Flowsheet

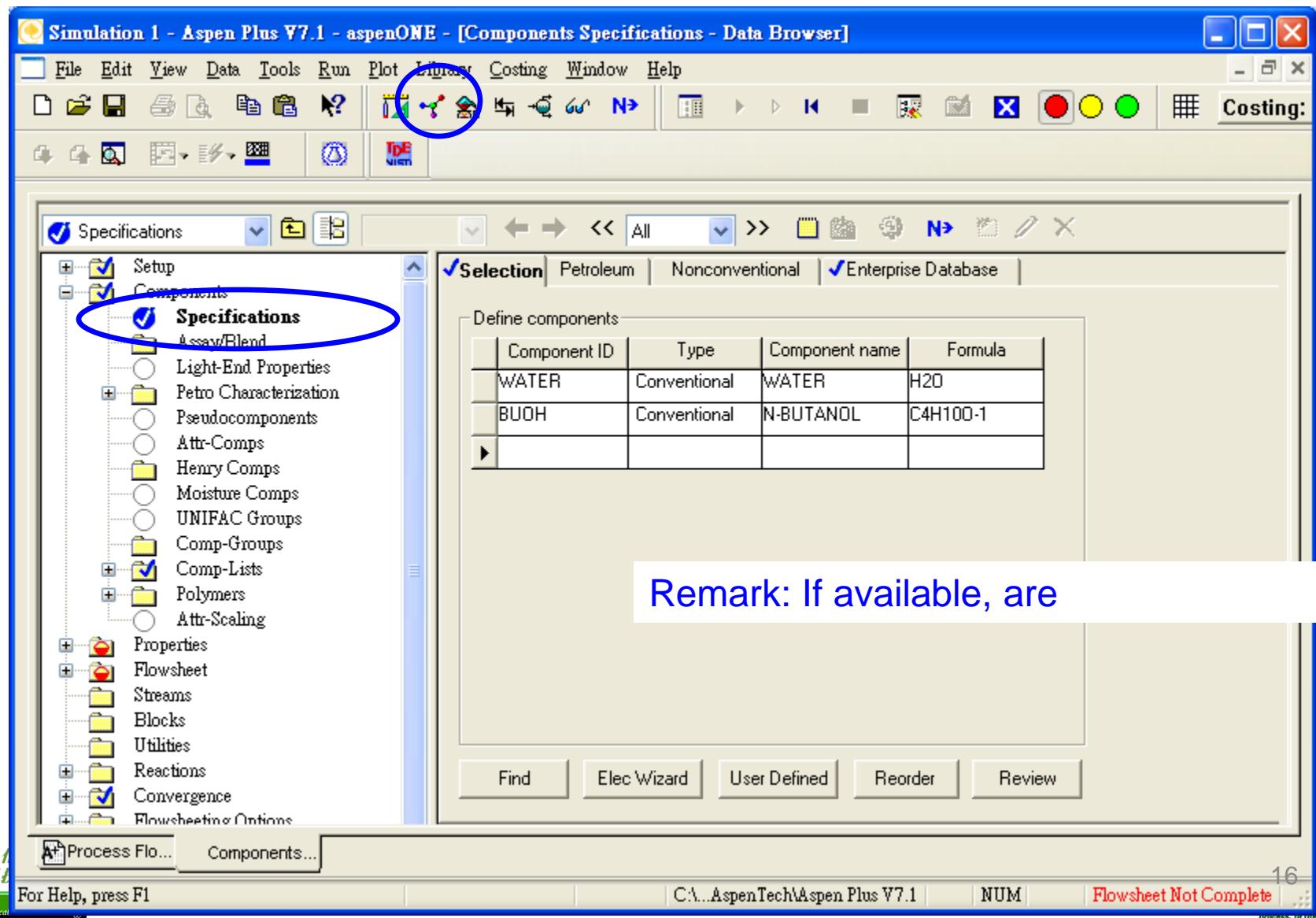
Assay Data Analysis
Data Regression
Flowsheet
Properties Plus
Property Analysis
Property Estimation

Input mode

Steady-State

Steady-State
Dynamic

Input components



The screenshot shows the Aspen Plus V7.1 interface with the title bar "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Components Specifications - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons, with the "Components" icon circled in blue. The left pane displays a tree view of simulation specifications, with the "Specifications" node circled in blue. The right pane shows a table titled "Define components" with two rows:

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H2O
BUOH	Conventional	N-BUTANOL	C4H10O-1

Below the table are buttons for Find, Elec Wizard, User Defined, Reorder, and Review. A blue text overlay at the bottom right reads "Remark: If available, are".

For Help, press F1

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Green Chemical

CA...AspenTech\Aspen Plus V7.1 | NUM | Flowsheet Not Complete | Intech

Properties

The screenshot shows the Aspen Plus 2006.5 software interface with the title bar "Simulation 1 - Aspen Plus 2006.5 - aspenONE - [Properties Specifications - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Window, and Help. The toolbar below has various icons for file operations, including a circled icon for properties.

The left pane displays a tree view of specifications:

- Setup (checked)
- Component (checked)
- Properties (checked)
- Specifications** (highlighted with a blue circle)
 - Property Methods (checked)
 - Estimation (checked)
 - Molecular Structure
 - Parameters (checked)
 - Data
 - Analysis
 - Prop-Sets (checked)
 - Advanced
 - CAPE-OPEN Packages
- Flowsheet
 - Streams
 - Blocks
 - Utilities
 - Reactions
 - Convergence (checked)
 - Flowsheeting Options
 - Model Analysis Tools
 - EO Configuration (checked)

The right pane shows the "Global" tab of the Properties Specifications dialog. It includes sections for Process type, Base method, Henry coefficients, Petroleum calculation options, Free-water method, Water solubility, Electrolyte calculation options, Chemistry ID, and Use true-components. A large blue arrow points from the "Specifications" node in the tree view to the "Process type" section of the dialog.

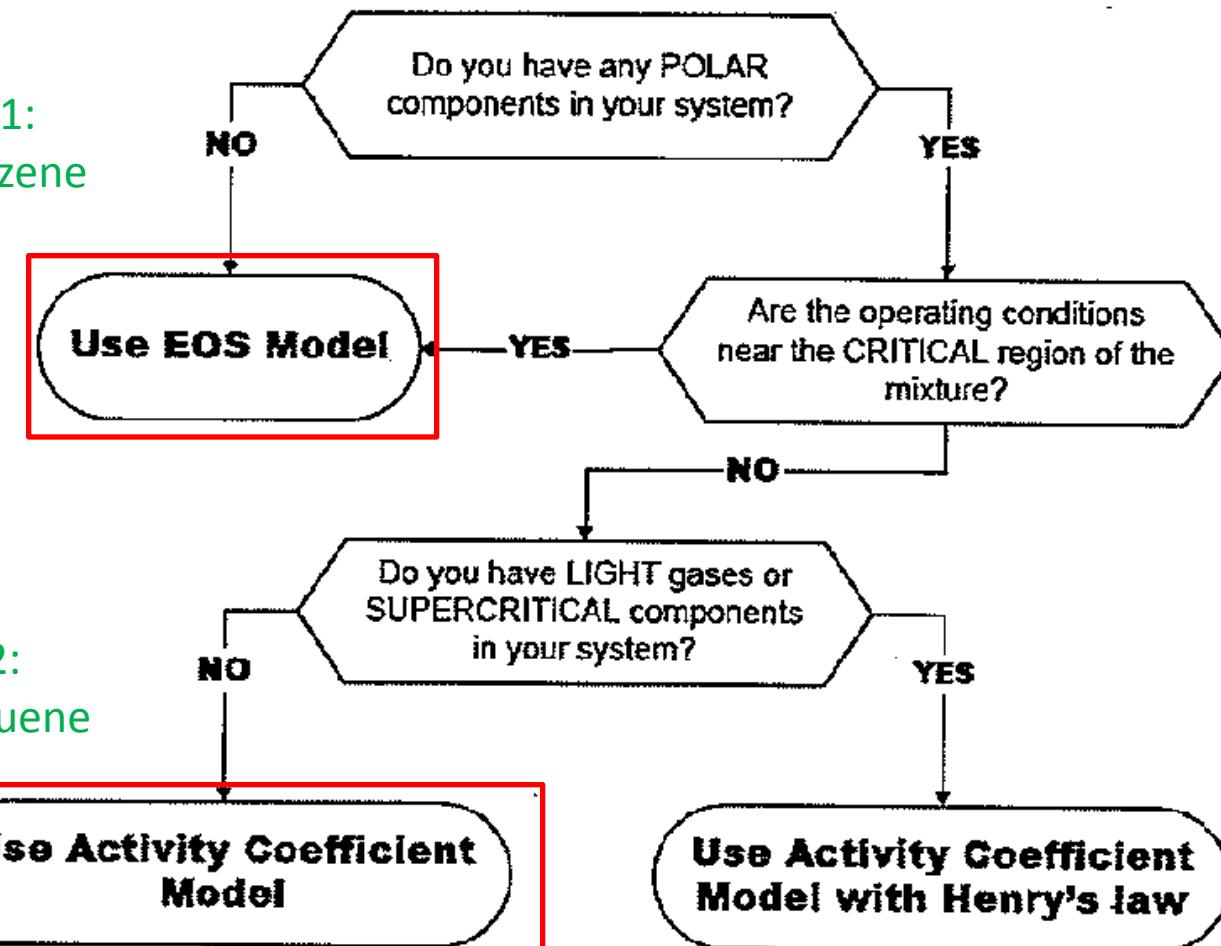
Process type(narrow the number of methods available)

Base method: IDEAL, NRTL, UNIQUAC, UNIFAC...

At the bottom, the status bar shows "For Help, press F1", "C:\..\penTech\Aspen Plus 2006.5", "NUM", "Flowsheet Not Complete", and a progress bar.

Property Method Selection—General Rule

Example 1:
water - benzene



Example 2:
benzene - toluene

Typical Activity Coefficient Models

Non-Random-Two Liquid Model (NRTL)

$$\ln \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ji}}{\sum_k x_k G_{ki}} \left[\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{ki}} \right]$$
$$G_{ij} = \exp(-\alpha_{ij} \tau_{ij}) \quad \tau_{ij} = a_{ij} + \frac{b_{ij}}{T} + e_{ij} \ln(T) + f_{ij} T$$
$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15K) \quad \tau_{ii} = 0 \quad G_{ii} = 1$$
$$a_{ij} \neq a_{ji} \quad b_{ij} \neq b_{ji} \quad c_{ij} \neq c_{ji} \quad d_{ij} \neq d_{ji}$$

Uniquac Model

$$\ln \gamma_i = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} - q'_i \ln t'_i - q'_i \sum_j \theta'_j \tau_{ij} / t'_j + \ell_i + q'_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j$$
$$\vdots$$

Unifac Model

$$\ln \gamma_i = \ln \gamma_i^c + \ln \gamma_i^r \quad \ln \gamma_i^r = \sum_k^{ng} \nu_{ki} [\ln \Gamma_k - \ln \Gamma_k^i]$$
$$\ln \gamma_i^c = \ln \left(\frac{\Phi_i}{x_i} \right) + 1 - \frac{\Phi_i}{x_i} - \frac{Z}{2} \left[\ln \left(\frac{\Phi_i}{\theta_i} \right) + 1 - \frac{\Phi_i}{\theta_i} \right]$$
$$\Phi_i = \frac{x_i r_i}{\sum_j^{nc} x_j r_j} \quad \theta_i = \frac{x_i \frac{z}{2} q_i}{\sum_j^{nc} x_j \frac{z}{2} q_j} \quad (\text{molecular volume and surface fractions})$$
$$r_i = \sum_k^{ng} \nu_{ki} R_k \quad q_i = \sum_k^{ng} \nu_{ki} Q_k \quad (R_k: \text{group volume}; Q_k: \text{area}) \dots$$

Typical Equation of States

Peng-Robinson (PR) EOS

$$\begin{aligned}P &= \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)} \\a &= \sum_i \sum_j x_i x_j \sqrt{a_i a_j} (1 - k_{ij}) \\b &= \sum_i x_i b_i \quad k_{ij} = k_{ji} \\a_i &= \text{fcn}(T, T_{ci}, P_{ci}, \omega_i) \quad b_i = \text{fcn}(T_{ci}, P_{ci})\end{aligned}$$

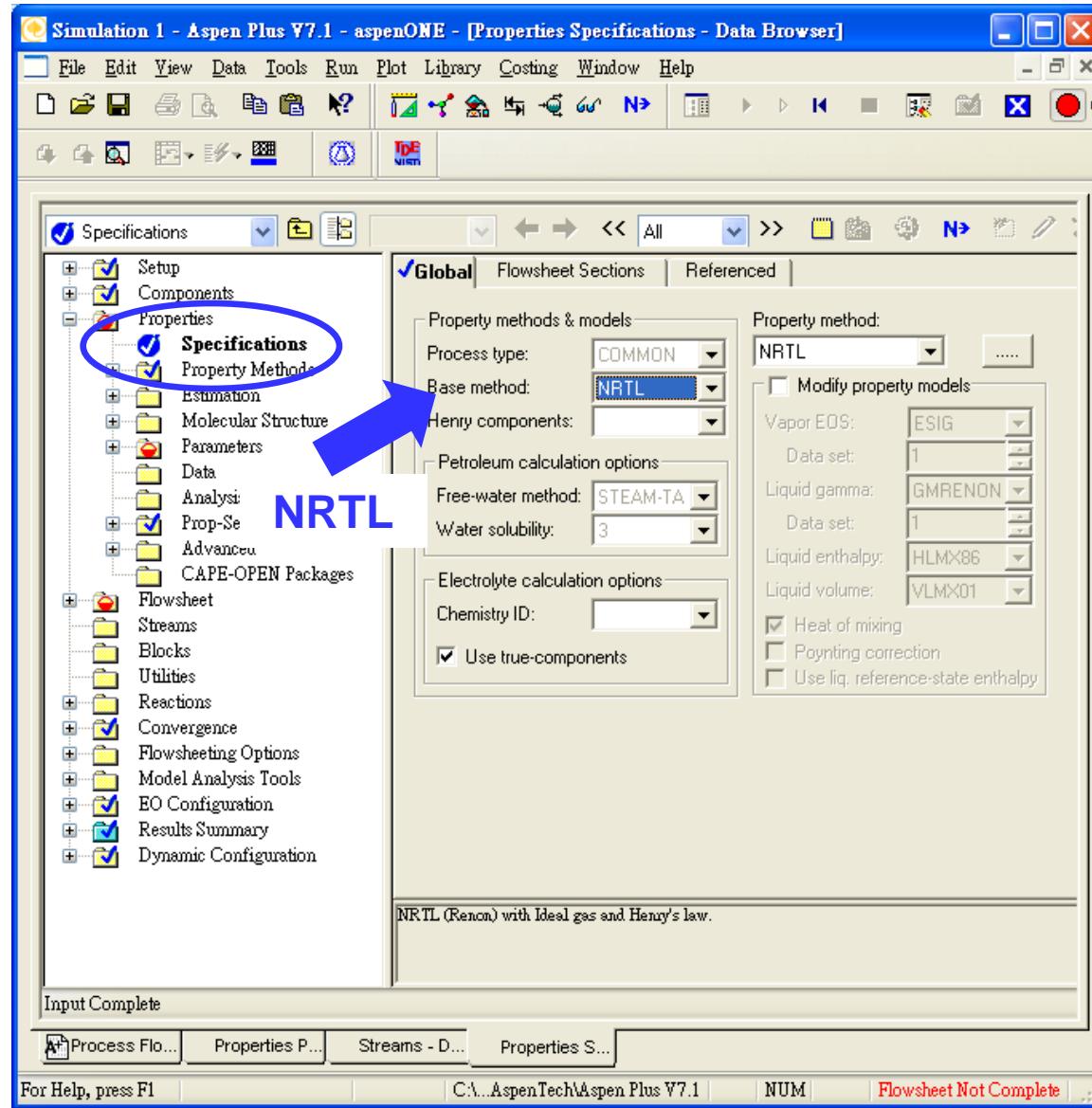
Redlich-Kwong (RK) EOS

$$\begin{aligned}P &= \frac{RT}{V-b} - \frac{a/\sqrt{T}}{V(V+b)} \\a &= \sum_i x_i \sqrt{a_i} \quad a_i = 0.42748023 R^2 T_{ci}^{1.5} / P_{ci} \\b &= \sum_i x_i b_i \quad b_i = 0.08664035 R T_{ci} / P_{ci}\end{aligned}$$

Haydon O'Connell (HOC) EOS

$$\begin{aligned}Z &= 1 + \frac{B}{RT} \\B &= \sum_i \sum_j x_i x_j B_{ij}(T) \\B_{ij} &= (B_{\text{free-nonpolar}})_{ij} + (B_{\text{free-polar}})_{ij} + (B_{\text{metastable}})_{ij} + (B_{\text{bound}})_{ij} + (B_{\text{chem}})_{ij} \\&\vdots\end{aligned}$$

Thermodynamic Model – NRTL



NRTL – Binary Parameters

The screenshot displays two software windows side-by-side. On the left is the 'Simulation 1 - Aspen Plus 2006.5 - aspenONE' window. Its interface includes a toolbar at the top, a menu bar with File, Edit, View, Data, Tools, Run, Plot, Library, Window, Help, and a main panel with a tree view under 'Specifications'. The 'Properties' node is expanded, showing 'Pure Component', 'Binary Interaction', and 'Electrolyte Pair' under 'Components'. A blue arrow points from the 'Binary Interaction' node to the right window. On the right is the 'Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Binary Interaction NRTL-1 (T-D...]' window. It has its own toolbar and menu bar. The main area shows a tree view under 'NRTL-1' with nodes like 'Setup', 'Components', 'Properties', 'Specifications', 'Property Methods', 'Estimation', 'Molecular Structure', and 'Parameters'. Under 'Parameters', 'Pure Component' is checked, and 'Binary Interaction' is also checked. Within 'Binary Interaction', 'NRTL-1' is selected. To the right of the tree view is a table titled 'Temperature-dependent binary parameters' with columns for 'Component i' and 'Component j'. The table lists several entries, with 'NRTL-1' highlighted by a blue circle.

Click “NRTL” and then built-in binary parameters appear automatically if available.

Access Properties Models and Parameters

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Components Specifications - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Costing:

Specifications

Selection Petroleum Nonconventional Enterprise Database

Define components

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H2O
BUOH	Conventional	N-BUTANOL	C4H10O-1

Review Databank Data

Find Elec Wizard User Defined Reorder Review

Process Flow Components...

For Help, press F1 C:\...AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

enTech

Review Databank Data

Including:

- Ideal gas heat of formation at 298.15 K
- Ideal gas Gibbs free energy of formation at 298.15 K
- Heat of vaporization at TB
- Normal boiling point
- Standard liquid volume at 60°F
- ...

The screenshot shows the Aspen Plus V7.1 interface. On the left, the 'Parameters' tree is displayed under 'REVIEW-1'. A blue circle highlights the 'REVIEW-1' node. The 'Input' tab is selected, showing a table titled 'Pure component scalar parameters'. A large blue oval surrounds the table area. The table lists various parameters for two components: WATER and BUOH. The parameters include API, CHARGE, DGFORM, DGSFRM, DHFORM, DHSFRM, DHVLB, FREEZEPT, HCOM, MUP, and MW. The table has columns for Parameters, Units, Data set, Component (for WATER), Component (for BUOH), and Component (empty). The 'Process Flow' and 'Properties P...' buttons are visible at the bottom.

Parameters	Units	Data set	Component (WATER)	Component (BUOH)	Component
API		1	10.00000000	42.40000000	
CHARGE		1		0.0	
DGFORM	kcal/mol	1	-54.59778351	-35.99407662	
DGSFRM	kcal/mol	1	-56.54915449		
DHFORM	kcal/mol	1	-57.75628165	-65.70650616	
DHSFRM	kcal/mol	1	-69.96274004		
DHVLB	kcal/mol	1	9.744506544	10.26946594	
FREEZEPT	C	1	0.0	-89.30000000	
HCOM	kcal/mol	1		-586.1278303	
MUP	debye	1	1.849723721	1.669847043	
MW		1	18.01528000	74.12280000	

Description of each parameter

Pure Component Temperature-Dependent Properties

The screenshot shows the Aspen Plus V7.1 Data Browser interface. The title bar reads "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Pure Component REVIEW-1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks. The left pane displays a tree view of parameters under "REVIEW-1", with "Pure Component" expanded, showing items like ATOMNO-1, CPIGDP-1, CPSDIP-1, DHVLDP-1, DNLDIP-1, DNSDIP-1, KLDIP-1, KV_DIP-1, MULDIP-1, MUVDIP-1, NOATOM-1, PLXANT-1, REVIEW-1, SIGDIP-1, UFGRP-1, UFGRPD-1, and UFGRPL-1. A blue oval highlights the "Pure Component" node. The right pane is a table titled "Parameter value." with the following entries:

CPIGDP-1	ideal gas heat capacity
CPSDIP-1	Solid heat capacity
DNLDIP-1	Liquid density
DHVLDP-1	Heat of vaporization
PLXANT-1	Extended Antoine Equation
MULDIP	Liquid viscosity
KLDIP	Liquid thermal conductivity
SIGDIP	Liquid surface tension
UFGRP	UNIFAC functional group

At the bottom, tabs for "Process Flow..." and "Properties P..." are visible, along with status bars for "C:\...AspenTech\Aspen Plus V7.1", "NUM", and "Flowsheet Not Complete".

Example: PLXANT-1 (Extended Antoine Equation)

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Pure Component PLXANT-1 - D...]

File Edit View Data Tools Run Plot Library Costing Window Help

Click “?” and then click where you don’t know

Parameters

- Pure Component
 - ATOMNO-1
 - CPIGDP-1
 - CPSDIP-1
 - DHVLDP-1
 - DNLDIP-1
 - DNSDIP-1
 - KLDIP-1
 - KVDIP-1
 - MULDIP-1
 - MUVDIP-1
 - NOATOM-1
 - PLXANT-1**
 - REVIEW-1
 - SIGDIP-1
 - UFGRP-1
 - UFGRPD-1
 - UFGRPL-1
- Binary Interaction
- Electrolyte Pair
- Electrolyte Ternary
- UNIFAC Group
- UNIFAC Group Binary
- Results
- Data
- Analysis
- Process Flow...
- Properties P...

Input Complete

Parameter: PLXANT Data set: []

Temperature-dependent correlation parameters

Components	WATER	BUOH
Temperature units	C	C
Property units	bar	bar
1	62.13607454	94.77707454
2	-7258.200000	-9866.400000
3	0.0	0.0
4	0.0	0.0
5	-7.303700000	-11.65500000
6	4.16530000E-6	1.0832000E-17
7	2.000000000	6.000000000
8	.0100000000	-89.30000000
9	373.9500000	289.9500000

Corresponding Model

APrSystem

Extended Antoine Equation

Parameters for many components are available for the extended Antoine equation from the Aspen Physical Property System pure component databank. This equation can be used whenever the parameter PLXANT is available.

The equation for the extended Antoine vapor pressure model is:

$$\ln p_i^{*j} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i} \ln T + C_{6i} T^{C_{7i}} \text{ for } C_{8i} \leq T \leq C_{9i}$$

Extrapolation of $\ln p_i^{*j}$ versus $1/T$ occurs outside of temperature bounds.

Parameter Name / Element	Symbol	Default	MDS	Lower Limit	Upper Limit	Units
PLXANT/1	C_{1i}		x			PRESSURE, TEMPERATURE
PLXANT/2	C_{2i}		x			TEMPERATURE
PLXANT/3, ..., 7	C_{3i}, \dots, C_{7i}	0	x			TEMPERATURE
PLXANT/8	C_{8i}	0	x			TEMPERATURE
PLXANT/9	C_{9i}	1000	x			TEMPERATURE

If C_{5i} , C_{6i} , or C_{7i} is non-zero, absolute temperature units are assumed for all coefficients C_{1i} through C_{7i} . The temperature limits are always in user input units.

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Example: CPIGDP-1 (Ideal Gas Heat Capacity Equation)

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Pure Component CPIGDP-1 - Da...]

File Edit View Data Tools Run Plot Library Costing Window Help

CPIGDP-1

Parameters

- Pure Component
 - ATOMNO-1
 - CPIGDP-1**
 - CPSDIP-1
 - DHVLDP-1
 - DNLDIP-1
 - DNSDIP-1
 - KLDIP-1
 - KVDIP-1
 - MULDIP-1
 - MUVDIP-1
 - NOATOM-1
 - PLXANT-1
 - REVIEW-1
 - SIGDIP-1
 - UFGRPD-1
 - UFGRPL-1
- Binary Interaction
- Electrolyte Pair
- Electrolyte Ternary
- UNIFAC Group
- UNIFAC Group Binary
- Results

Data Analysis Prop. Sets

Input Complete

Process Flow... Properties P...

File Help, press F1 C:\AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

Corresponding Model

APrSystem

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Aspen Ideal Gas Heat Capacity Polynomial

The ideal gas heat capacity polynomial is available for components stored in ASPENPCD, AQUEOUS, and SOLIDS databanks. This model is also used in PCES.

$C_p^{*ig} = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 + C_{6i}T^5$ for $C_{7i} \leq T \leq C_{8i}$

$C_p^{*ig} = C_{9i} + C_{10i}T^{C_{11i}}$ for $T < C_{7i}$

C_p^{*ig} is [linearly extrapolated](#) using slope at C_{8i} for $T > C_{8i}$

Parameter Name/Element	Symbol	Default	MDS	Lower Limit	Upper Limit	Units
CPIG/1	C_{1i}	—	—	—	—	MOLE-HEAT-CAPAC TEMPERATURE
CPIG/2, ..., 6	C_{2i}, \dots, C_{6i}	0	—	—	—	MOLE-HEAT-CAPAC TEMPERATURE
CPIG/7	C_{7i}	0	—	—	—	TEMPERATURE
CPIG/8	C_{8i}	1000	—	—	—	TEMPERATURE
CPIG/9, 10, 11	C_{9i}, C_{10i}, C_{11i}	—	—	—	—	MOLE-HEAT-CAPAC TEMPERATURE †

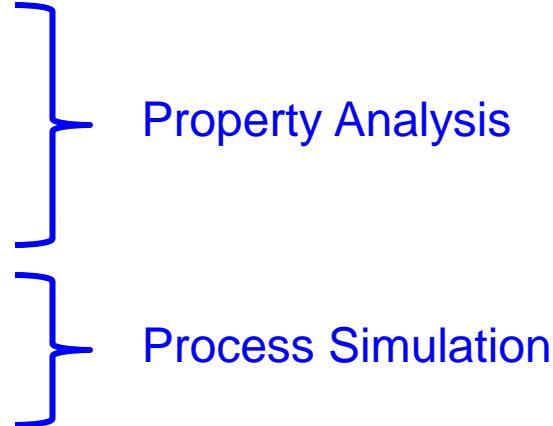
† If C_{10i} or C_{11i} is non-zero, then [absolute temperature units](#) are assumed for C_{9i} through C_{11i} . Otherwise, user input temperature units are used for all parameters. User input temperature units are always used for C_{1i} through

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Basic Input---Summary

- The minimum **required inputs** to run a simulation are:

- Setup
- Components
- Properties
- Streams
- Blocks



Introduction to Aspen Plus

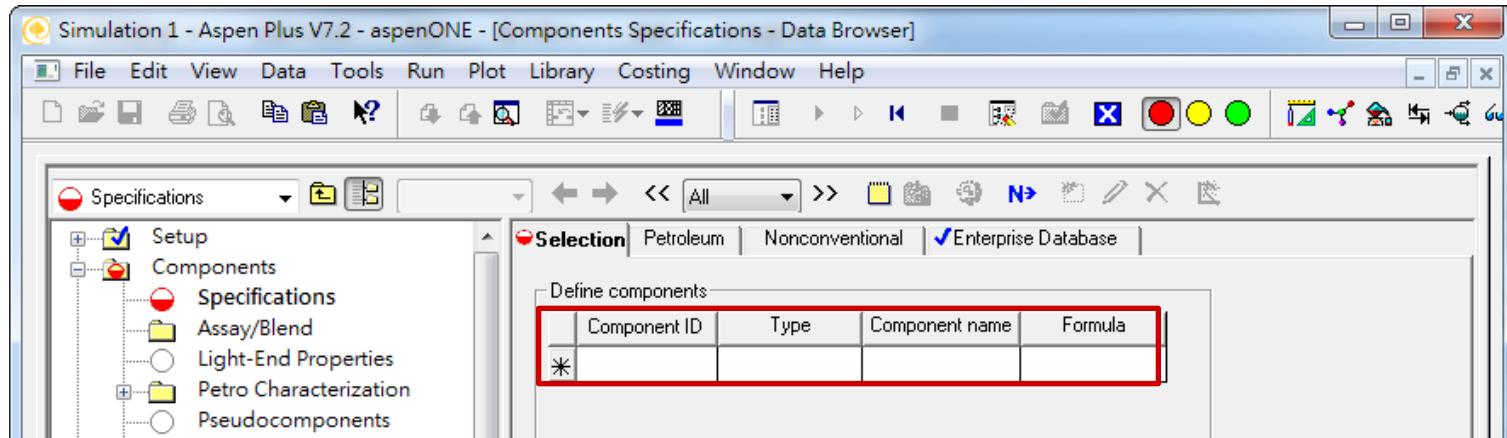
Part 3: Property analysis

Overview of Property Analysis

Use this form	To generate
Pure	Tables and plots of pure component properties as a function of temperature and pressure
Binary	Txy, Pxy, or Gibbs energy of mixing curves for a binary system
Residue	Residue curve maps
Ternary	Ternary maps showing phase envelope, tie lines, and azeotropes of ternary systems
Azeotrope	This feature locates all the azeotropes that exist among a specified set of components.
Ternary Maps	Ternary diagrams in Aspen Distillation Synthesis feature: Azeotropes, Distillation boundary, Residue curves or distillation curves, Isovatility curves, Tie lines, Vapor curve, Boiling point

***When you start properties analysis, you **MUST** specify **components** , **thermodynamic model** and **its corresponding parameters**. (Refer to Part 2)

Find Components

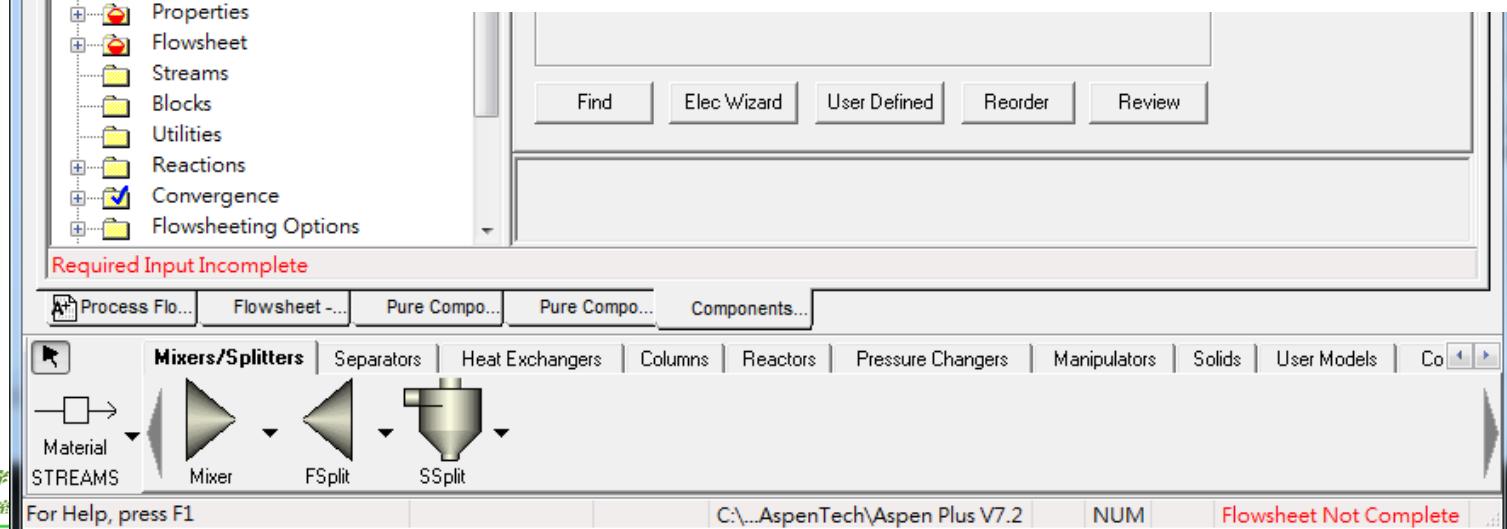


Component ID : just for distinguishing in Aspen.

Type : Conventional, Solid....etc

Component name : real component name

Formula : real component formula



Find Components

The screenshot shows the Aspen Plus V7.2 interface. The title bar reads "Simulation 1 - Aspen Plus V7.2 - aspenONE - [Components - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks. On the left, a tree view under "Components" shows categories like Setup, Components, Assay/Blend, Petro Characterization, Pseudocomponents, Attr-Comps, Henry Comps, Moisture Comps, UNIFAC Groups, Comp-Groups, Comp-Lists, Polymers, Attr-Scaling, Properties, and Parameters. Under Properties, "Pure Component" and "Binary Interaction" are checked. A message "Input Complete" is displayed at the bottom of the tree view. The main workspace is titled "Selection" and includes tabs for Petroleum, Nonconventional, and Enterprise Database. It features a "Define components" table:

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H2O
BUOH	Conventional	N-BUTANOL	C4H10O-1
*			

A red box highlights the "Component ID" column. Below the table, there is a "Find" button. To the right of the table, a tip is displayed:

TIP 1: For common components, you can enter directly the common name or molecular equation of the components in “component ID”.

(like water, CO2, CO, Chlorine...etc)

At the bottom, there are tabs for Process Flow and Components, and a toolbar with icons for Material STREAMS, Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and more. The status bar at the bottom shows "For Help, press F1", the path "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Flowsheet Not Complete".

Find Components

The screenshot shows the Aspen Plus V7.2 Components - Data Browser window. The left sidebar lists categories like Setup, Components, Properties, and others. The main area displays a table titled "Define components" with two rows:

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H2O
BUOH	Conventional	N-BUTANOL	C4H10O-1

A red box highlights the "Component name" column. A tip box in the center-right contains the following text:

TIP 2: If you know the component name (like N-butanol, Ethanol....etc), you can enter it in “component name”.

At the bottom, there are buttons for Find, Elec Wizard, User Defined, Reorder, and Review.

Below the table, there are tabs for Process Flow... and Components..., and icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT.

Find Components

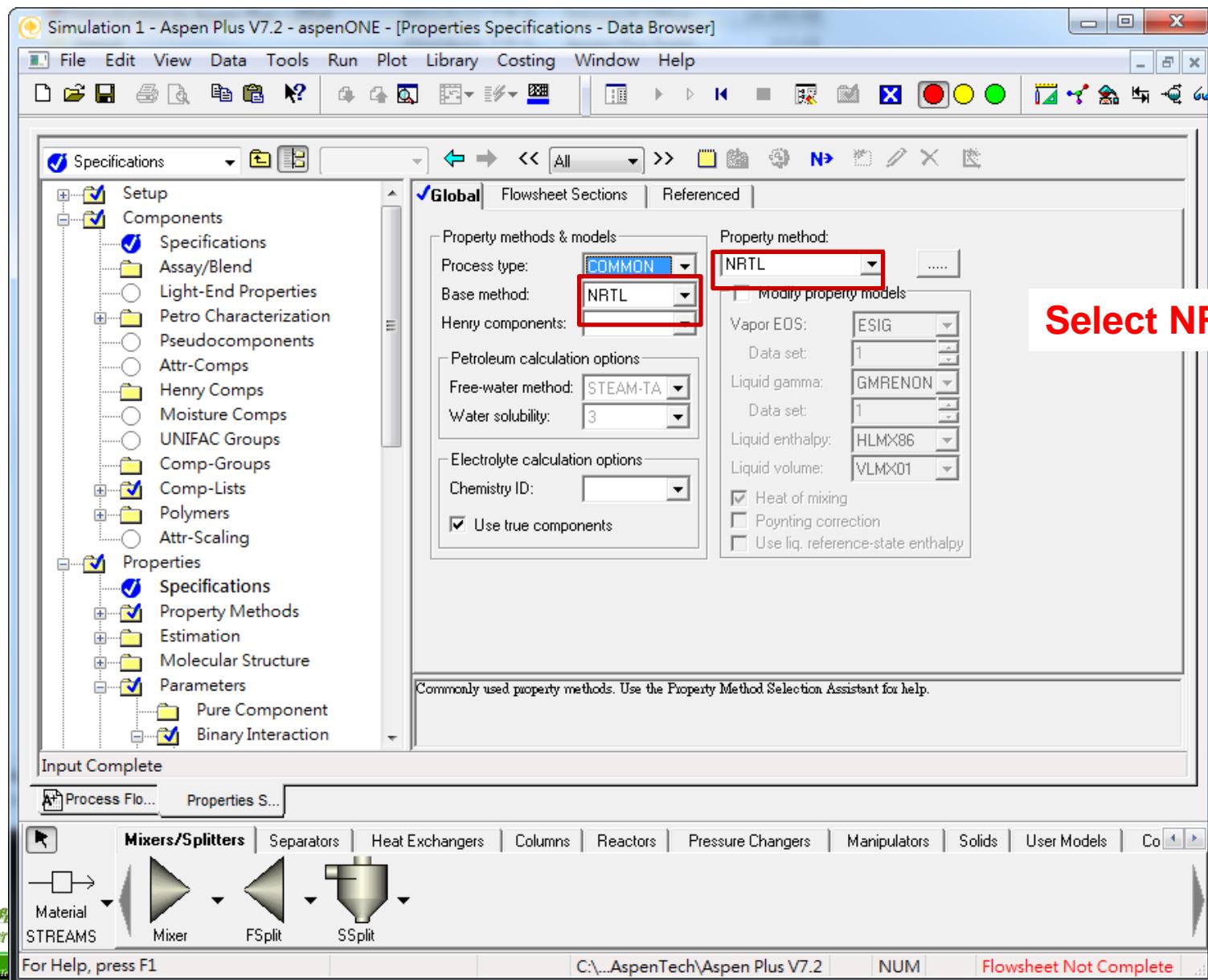
The screenshot shows the Aspen Plus V7.2 Components - Data Browser window. On the left is a tree view of component categories: Setup, Components (selected), Specifications, Assay/Blend, Light-End Properties, Petro Characterization, Pseudocomponents, Attr-Comps, Henry Comps, Moisture Comps, UNIFAC Groups, Comp-Groups, Comp-Lists, Polymers, Attr-Scaling, Properties, and Parameters. The Components category is expanded, showing Assay/Blend, Light-End Properties, Petro Characterization, Pseudocomponents, Attr-Comps, Henry Comps, Moisture Comps, UNIFAC Groups, Comp-Groups, Comp-Lists, Polymers, Attr-Scaling, and Properties. Under Properties, Specifications, Property Methods, Estimation, Molecular Structure, and Parameters are selected. The main area displays a table titled "Define components" with columns: Component ID, Type, Component name, and Formula. Two rows are present: WATER (Conventional, WATERT, H₂O) and BUOH (Conventional, N-BUTANOL, C₄H₁₀O-1). A red box highlights the "Formula" column. Below the table are buttons: Find (circled in blue), Elec Wizard, User Defined, Reorder, and Review. A green arrow points from the text "You can also click ‘Find’ to search for component of given CAS number, molecular weight without knowing its molecular formula, or if you don’t know the exactly component name" to the "Find" button.

TIP 3: You can also enter the formula of the component. (Be aware of the isomers)

You can also click “Find” to search for component of given CAS number, molecular weight without knowing its molecular formula, or if you don’t know the exactly component name

Component ID	Type	Component name	Formula
WATER	Conventional	WATERT	H ₂ O
BUOH	Conventional	N-BUTANOL	C ₄ H ₁₀ O-1
*			

Select Thermodynamic Model



Check Binary Parameter

Properties



Parameters



NRTL-1

The screenshot shows the Aspen Plus V7.2 interface. On the left, the 'Properties' tree is displayed under 'NRTL-1'. The 'Properties' node is selected and highlighted with a red box. Below it, the 'Binary Interaction' node is also highlighted with a red box. Under 'Binary Interaction', the 'NRTL-1' node is selected and highlighted with a red box. A green arrow points from this red box down towards the 'Input' tab on the right. The 'Input' tab shows the 'Parameter' set to 'NRTL' and the 'Data set' set to '1'. It displays 'Temperature-dependent binary parameters' for components WATER and BUOH. The table includes columns for Component i, Component j, Temperature units (F), Source (APV72 VLE-IG), Property units, and numerical values for AIJ, AJI, BIJ, and BJI. A checkbox at the bottom left of the tab is labeled 'Estimate missing parameters by UNIFAC'. At the bottom of the window, there are tabs for 'Process Flow...', 'Properties P...', and various process equipment icons like Mixers, Separators, Heat Exchangers, etc.

Properties

Parameters

NRTL-1

Input Complete

Process Flow... Properties P...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS Mixer FSplit SSplit

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Flowsheet Not Complete 36

Click This, it will automatically change to red if binary parameter exists.

Find Components

The screenshot shows the Aspen Plus V7.2 Components - Data Browser window. The left sidebar lists categories like Setup, Components, Properties, and others. The main area displays a table titled "Define components" with two rows:

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H2O
BUOH	Conventional	N-BUTANOL	C4H10O-1

A red box highlights the "Component name" column. A tip box in the center-right contains the following text:

TIP 2: If you know the component name (like N-butanol, Ethanol....etc), you can enter it in “component name”.

At the bottom, there are buttons for Find, Elec Wizard, User Defined, Reorder, and Review.

Below the table, there are tabs for Process Flow... and Components..., and a toolbar with icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT.

Find Components

You can enter
the way of
searching...

Find Compounds

Compounds Databanks

Search criteria

Compound name or formula or CAS number : begins with contains equals

Compound class :

MW From To
TB From To K

Find now New search Help

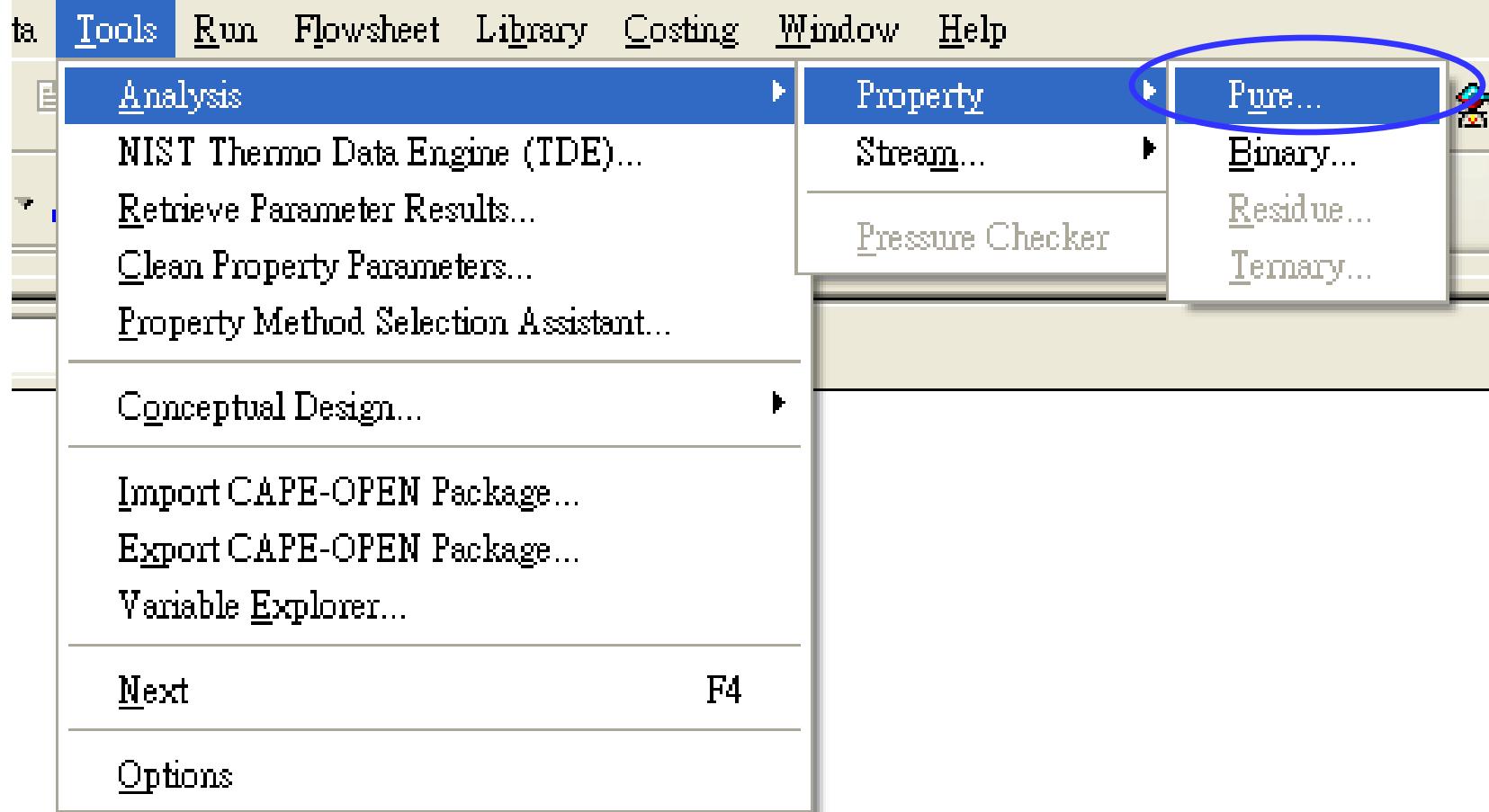
Compounds selected: 1

Compound name	Form...	Alternate name	CAS no	Compound class
2-ACETOACETOXY-ETHYL-MET...	C10H...	2-(3-OXOBUTA...	21282...	POLYFUNCTION...
N-BUTANOL	C4H1...	1-BUTANOL	71-36-3	N-ALCOHOLS
2-BUTANOL	C4H1...	(+)-2-BUTANOL	78-92-2	OTHER-ALIPH...
ISOBUTANOL	C4H1...	BUTANOL-ISO	78-83-1	OTHER-ALIPH...
TERT-BUTYL-ALCOHOL	C4H1...	BUTANOL TER...	75-65-0	OTHER-ALIPH...
2-AMINO-2-METHYL-1-PROPAN...	C4H1...	2-AMINOISOBU...		{
GAMMA-BUTYROLACTONE	C4H6...	1,2-BUTANOLIDE	96-48-0	OTHER-SATUR...
ACETALDOL	C4H8...	3-BUTANOLAL	107-8...	OTHER-POLYFU...
2-METHYL-1-BUTANOL	C5H1...	1-BUTANOL, 2...	137-3...	OTHER-ALIPH...

Add selected compounds Close

Properties Analysis – Pure Component

Plus V7.1 - aspenONE - [Process Flowsheet Window]



Available Properties

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Pure Component Properties Analysis]

Property (thermodynamic)	Property (transport)
Availability	Free energy
Constant pressure heat capacity	Enthalpy
Heat capacity ratio	Fugacity coefficient
Constant volume heat capacity	Fugacity coefficient pressure correction
Free energy departure	Vapor pressure
Free energy departure pressure correction	Density
Enthalpy departure	Entropy
Enthalpy departure pressure correction	Volume
Enthalpy of vaporization	Sonic velocity
Entropy departure	

Property type: Thermodynamic

Components: WATER, BUOH, BUAC

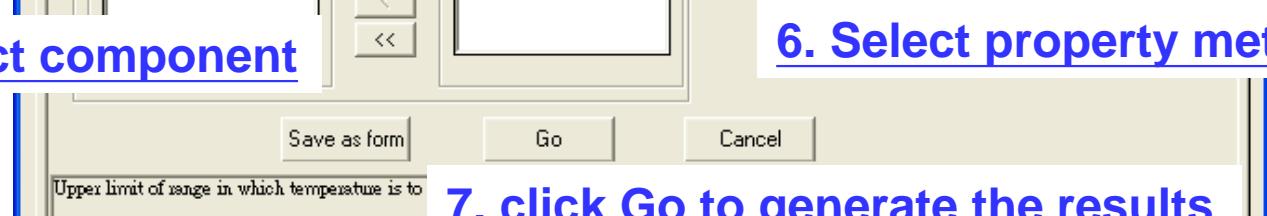
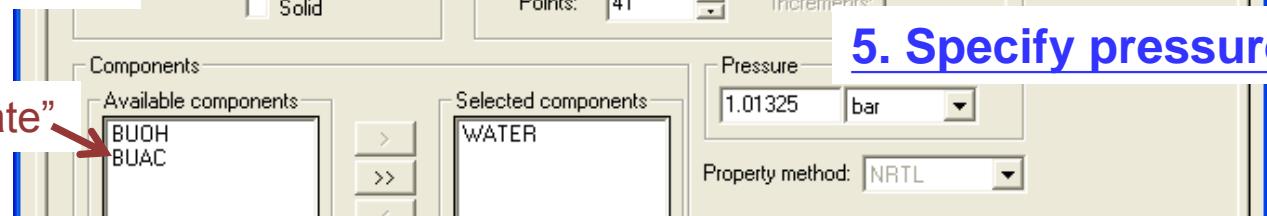
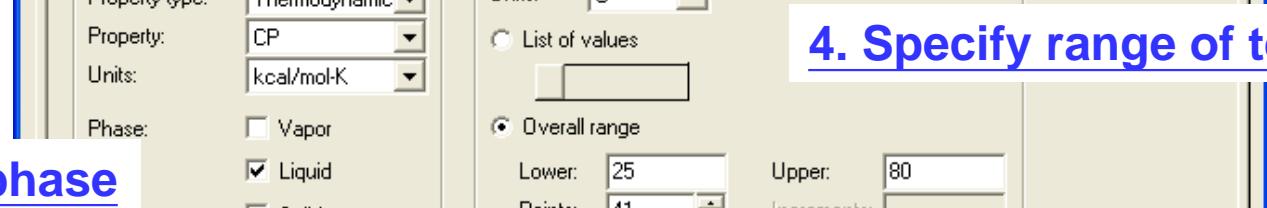
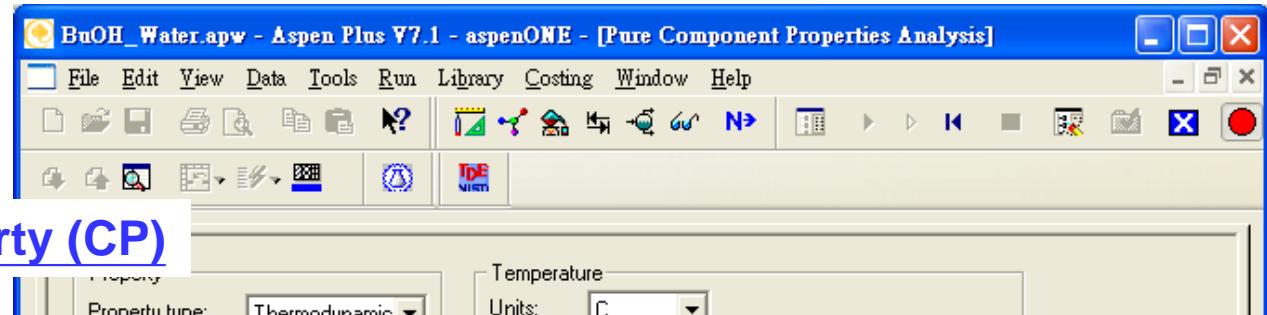
Property to be tabulated.

Process Flow... Pure Component...

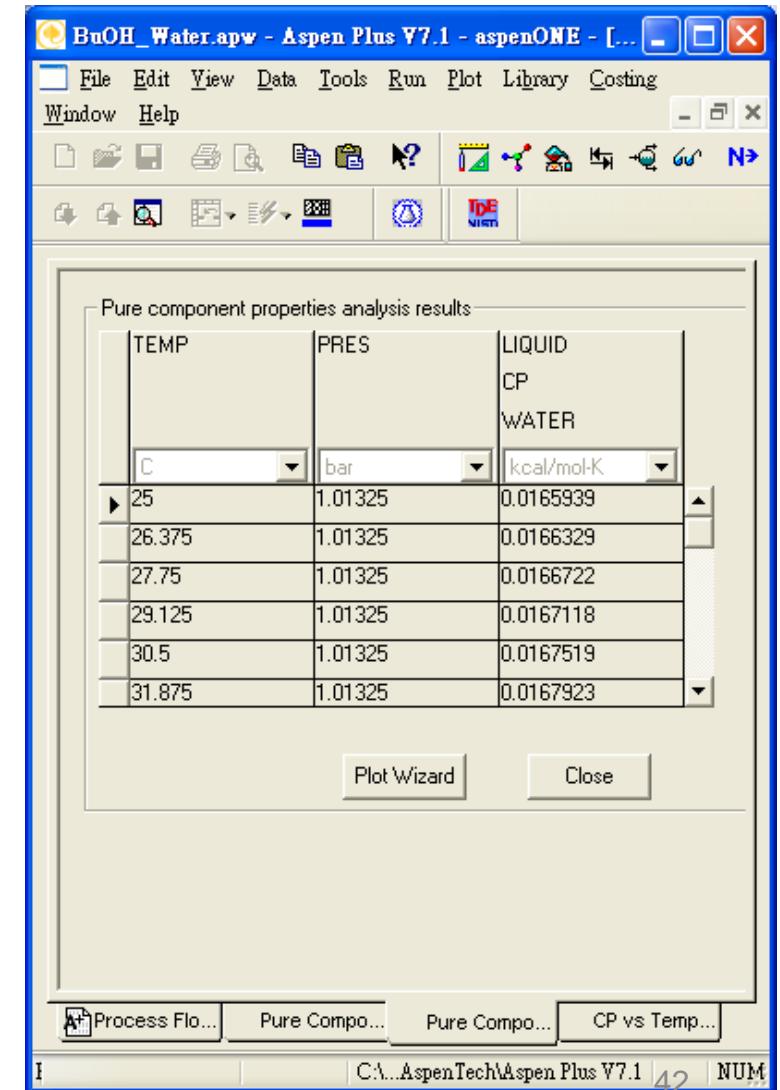
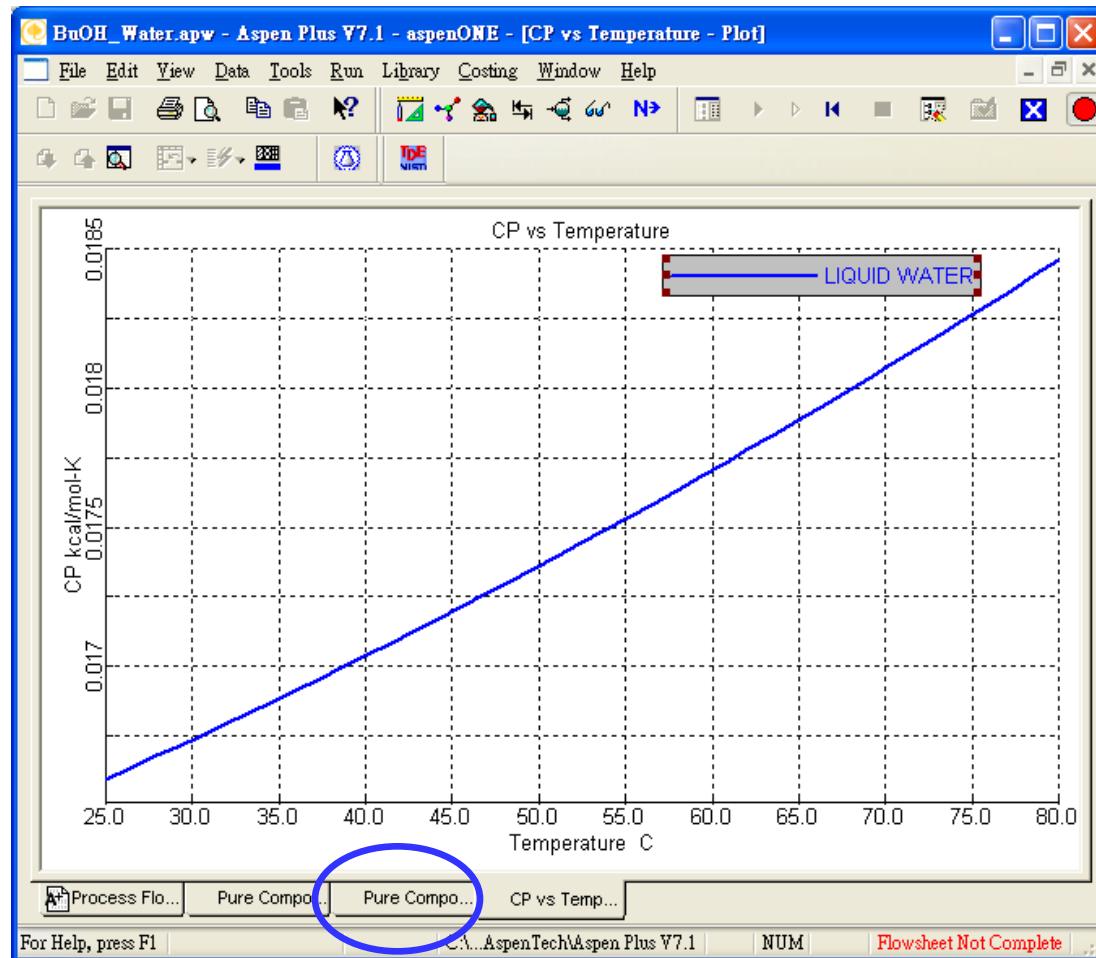
For Help, press F1 C:\...\AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

40

Example1: CP (Heat Capacity)

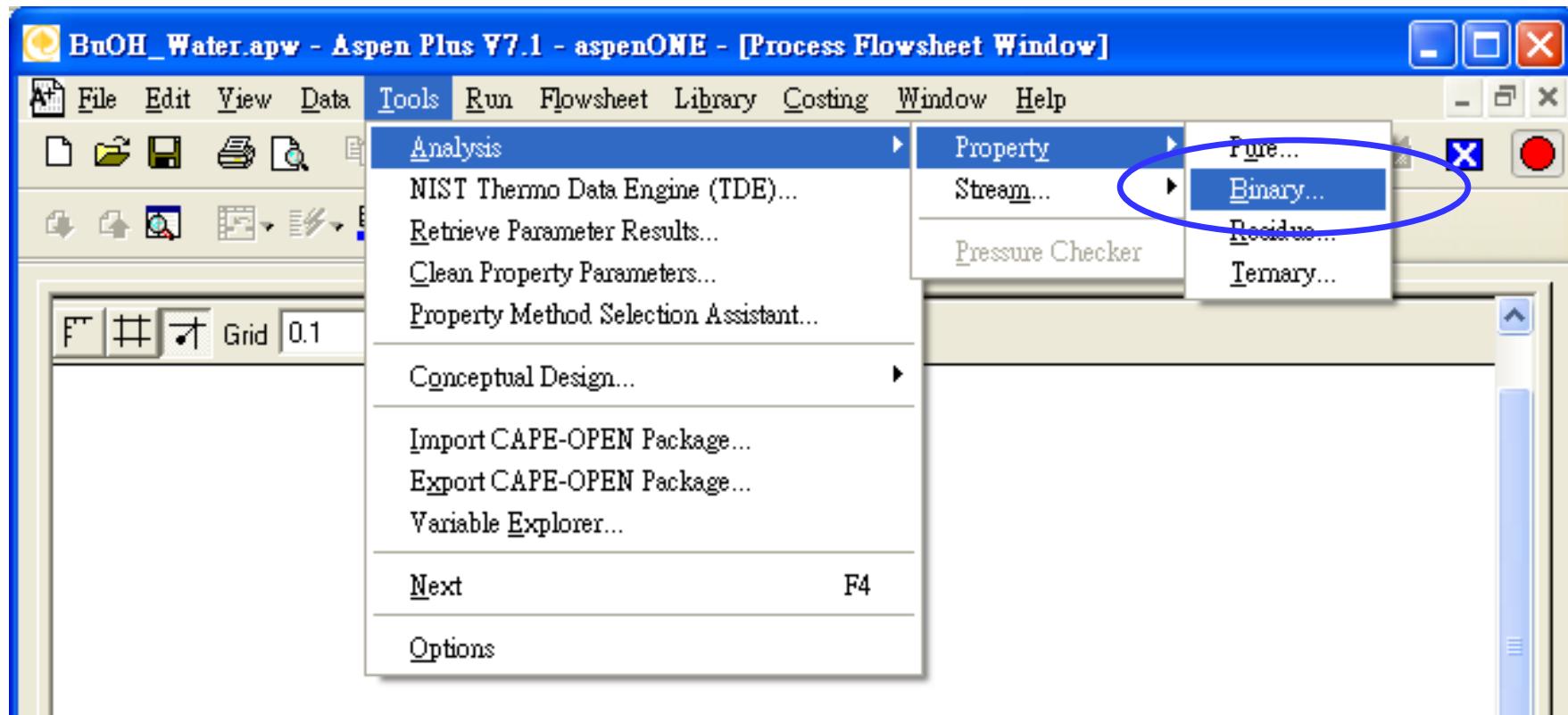


Example1: Calculation Results of CP



Data results

Properties Analysis – Binary Components



Binary Component Properties Analysis

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Binary Analysis]

File Edit View Data Tools Run Library Costing Window Help

Process Flow Binary Anal...

For Help, press F1 | C:\...AspenTech\Aspen Plus V7.1 | NUM | Flowsheet Not Complete

Use this Analysis type	To generate
Txy	Temperature-compositions diagram at constant pressure
Pxy	Pressure-compositions diagram at constant temperature
Gibbs energy of mixing	Gibbs energy of mixing diagram as a function of liquid compositions. The Aspen Physical Property System uses this diagram to determine whether the binary system will form two liquid phases at a given temperature and pressure.

Analysis type: Txy
Components: BuOH, WATER
Component 1: Gibbs energy of mixing
Component 2: BuOH
Compositions: Basis: Mole fraction, Component: WATER
Overall range: Lower: 0, Upper: 1, Points: 41, Increments:
Simulation approach: True species

Example: T-XY

1. Select analysis type (Txy)

Analysis type: Txy

Components

Component 1: WATER

Component 2: BUOH

2. Select two component

Compositions

Basis: Mole fraction

Component: WATER

3. Select compositions basis

Overall range

Lower: 0

Upper: 1

Points: 41

4. Specify composition range

2. Select phase (VLE, VLLE)

Valid phases

Vapor-Liquid-Liquid

Pressure

Units: bar

List of values

1.01325

Overall range

Lower:

Upper:

Points:

Increments:

5. Specify pressure

Property options

Property method: NRTL

Henry components:

Chemistry

6. Select property method

Simulation approach: True species

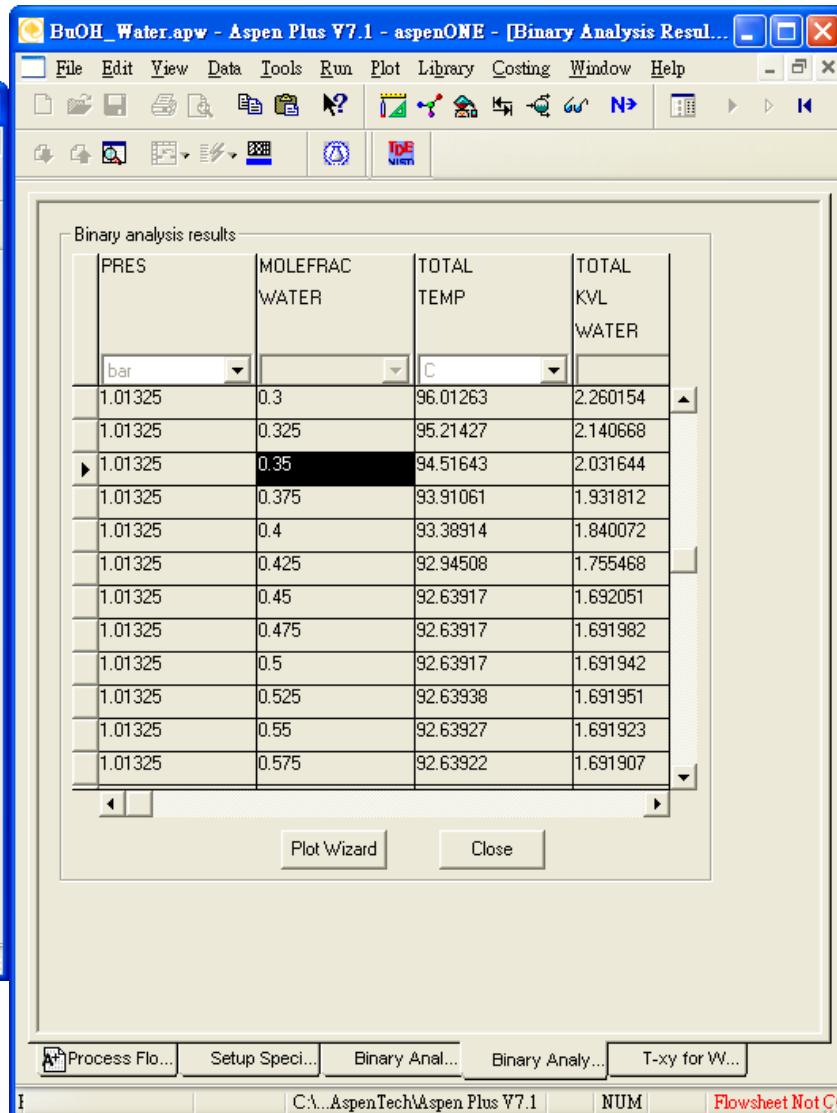
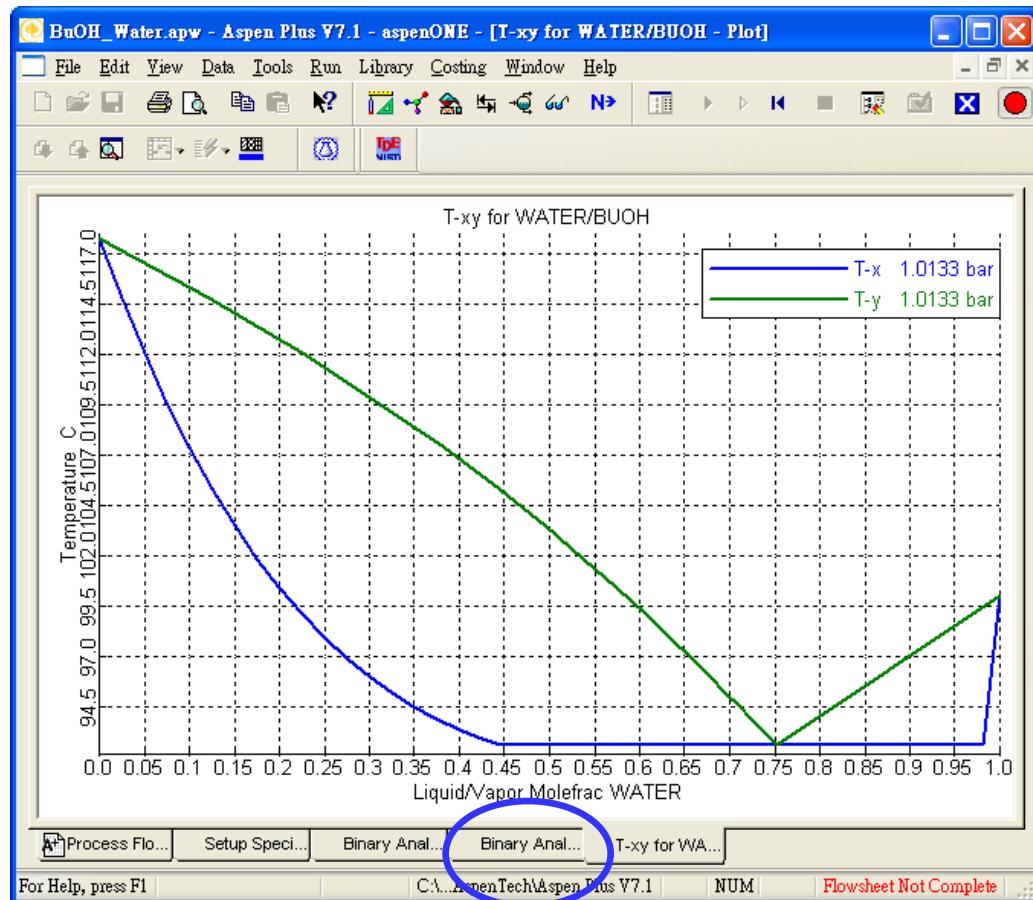
Save As Form

Go

Cancel

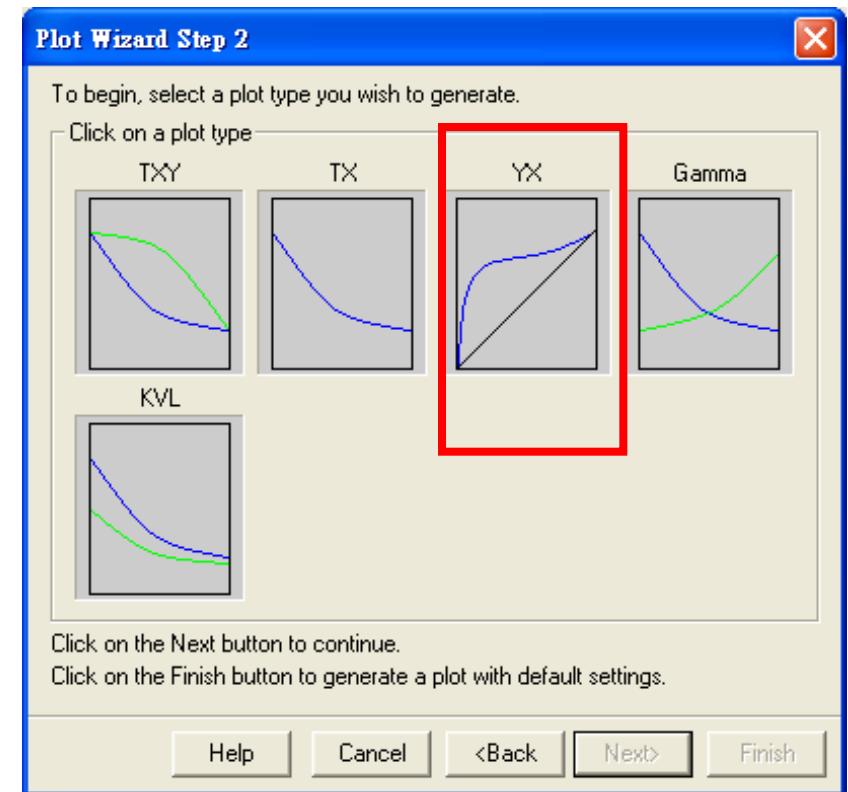
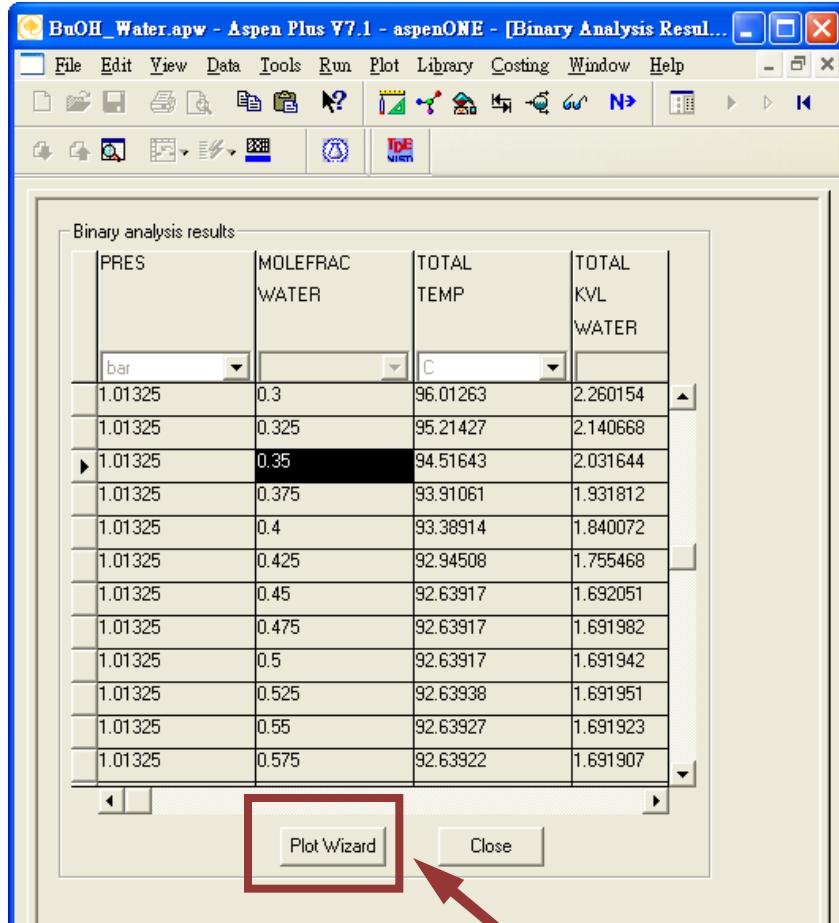
7. click Go to generate the results

Example: calculation result of T-XY

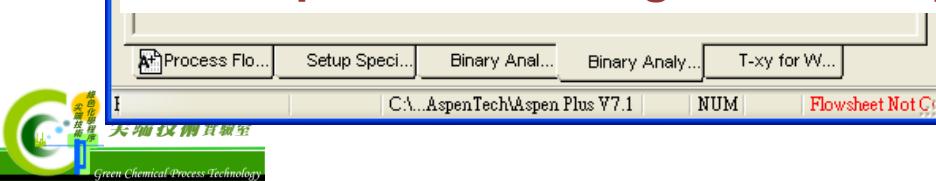


Data results

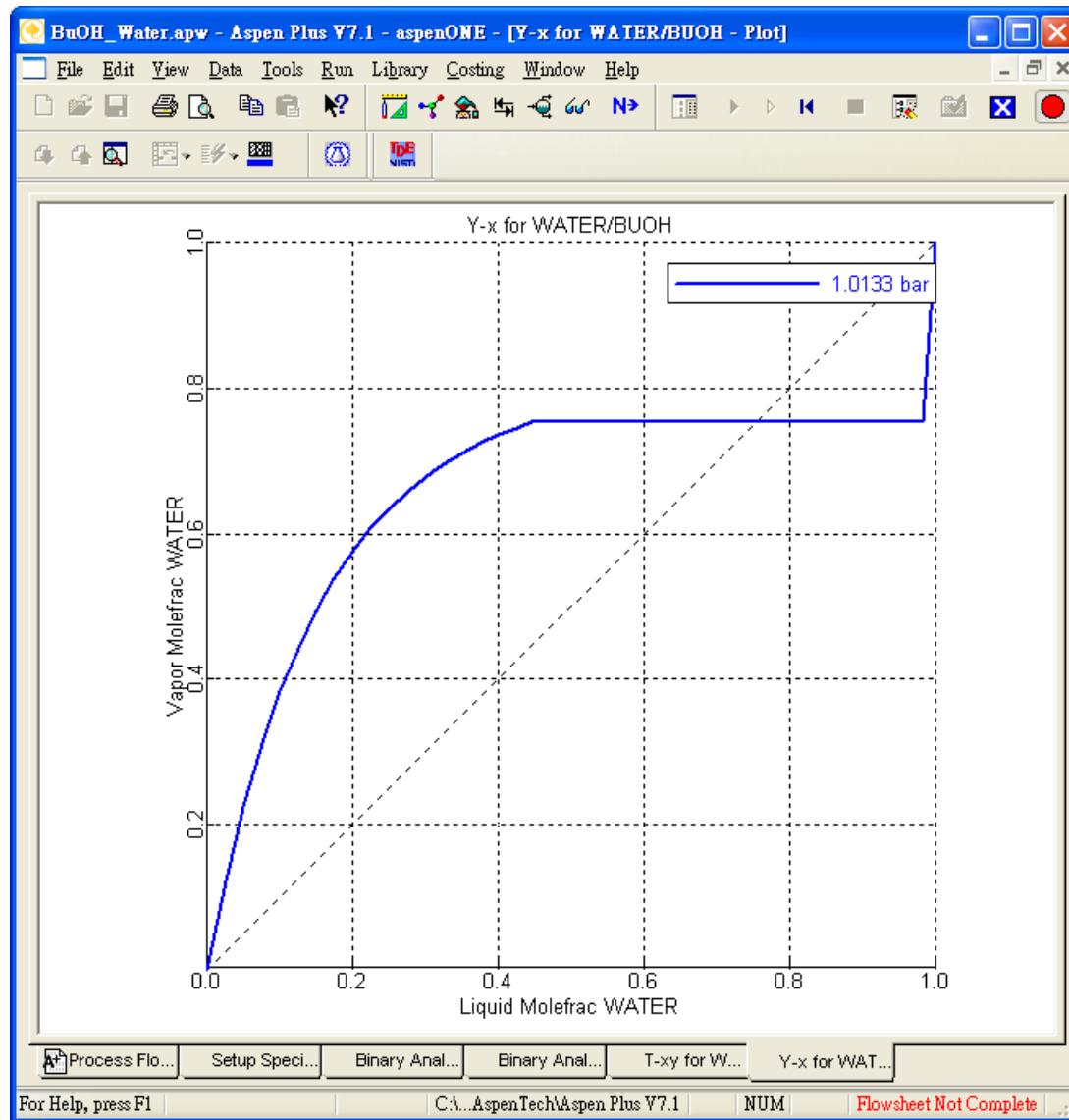
Example: Generate XY plot



Click “plot wizard” to generate XY plot



Example: Generate XY plot (cont'd)



Properties Analysis – Ternary (add one new components)

Simulation 1 - Aspen Plus V7.2 - aspenONE - [Components Specifications - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Specifications Selection Petroleum Nonconventional Enterprise Database

Define components

Component ID	Type	Component name	Formula
WATER	Conventional	WATER	H ₂ O
BUOH	Conventional	N-BUTANOL	C ₄ H ₁₀ O-1
BUAC	Conventional	N-BUTYL ACETATE	C ₆ H ₁₂ O ₂ -1

Find Elec Wizard User Defined Reorder Review

Input Complete

Process Flow Properties Properties Components

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS Mixer FSplit SSplit

aspenTech process... to the power of...

Properties Analysis – Ternary (Check NRTL binary parameter)

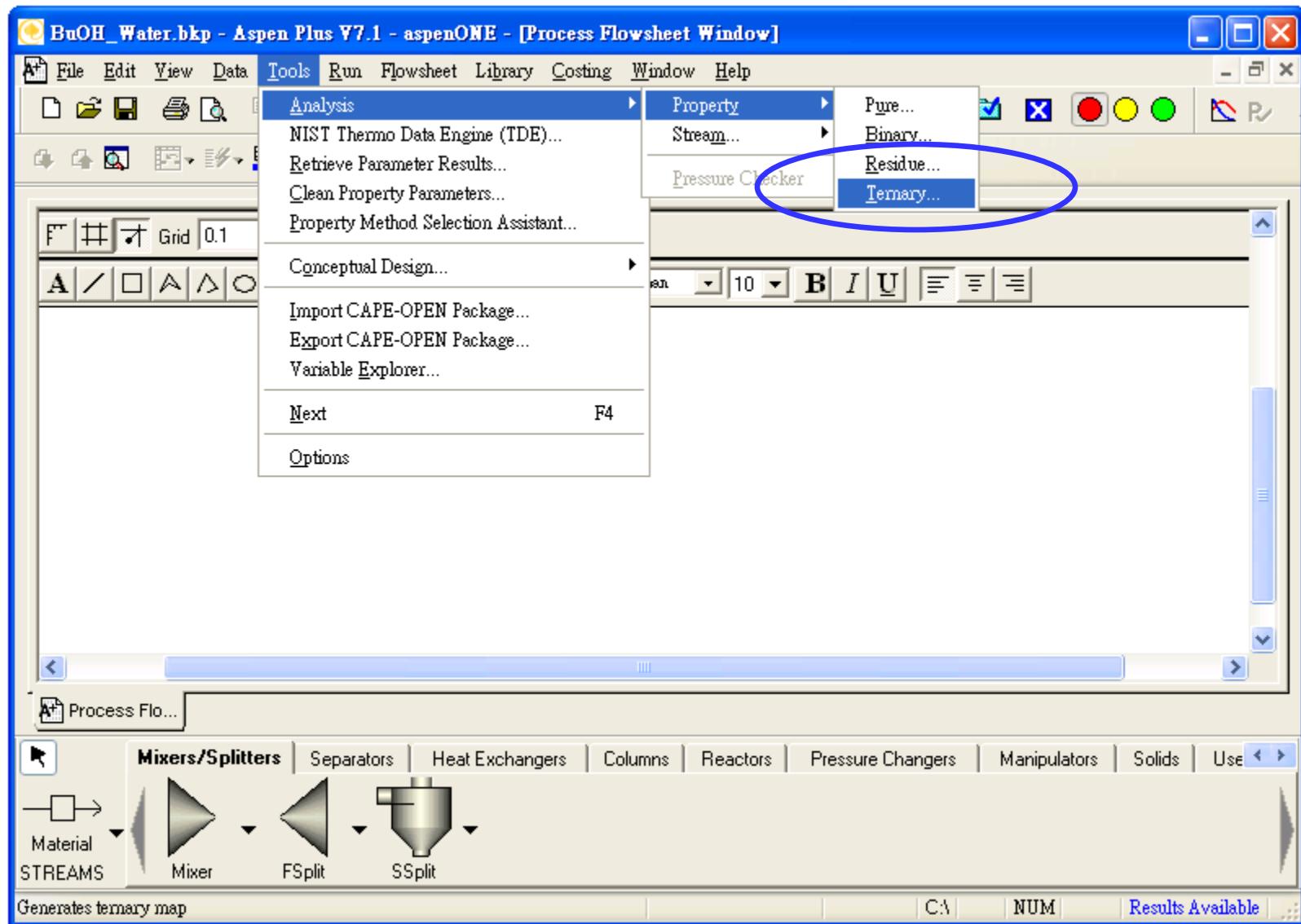
The screenshot shows the Aspen Plus interface with the following details:

- Left Sidebar:** Shows the project tree under "NRTL-1". Components listed include Petro Characterization, Pseudocomponents, Attr-Comps, Henry Comps, Moisture Comps, UNIFAC Groups, Comp-Groups, Comp-Lists, Polymers, Attr-Scaling, Properties, Specifications, Property Methods, Estimation, Molecular Structure, and Parameters. Under Parameters, Binary Interaction is selected, showing options like ANDKJU-1, ANDMUI-1, HENRY-1, NRTL-1, and RKTKU-1.
- Input Tab:** Set to "NRTL" and "Data set: 1".
- Table:** "Temperature-dependent binary parameters" for three components: WATER, BUOH, and BUAC. The table has columns for Component i, Temperature units (F), Source (APV72 VLE-IG), and Property units (AJJ, AJI, BIJ, BJI). The data is as follows:

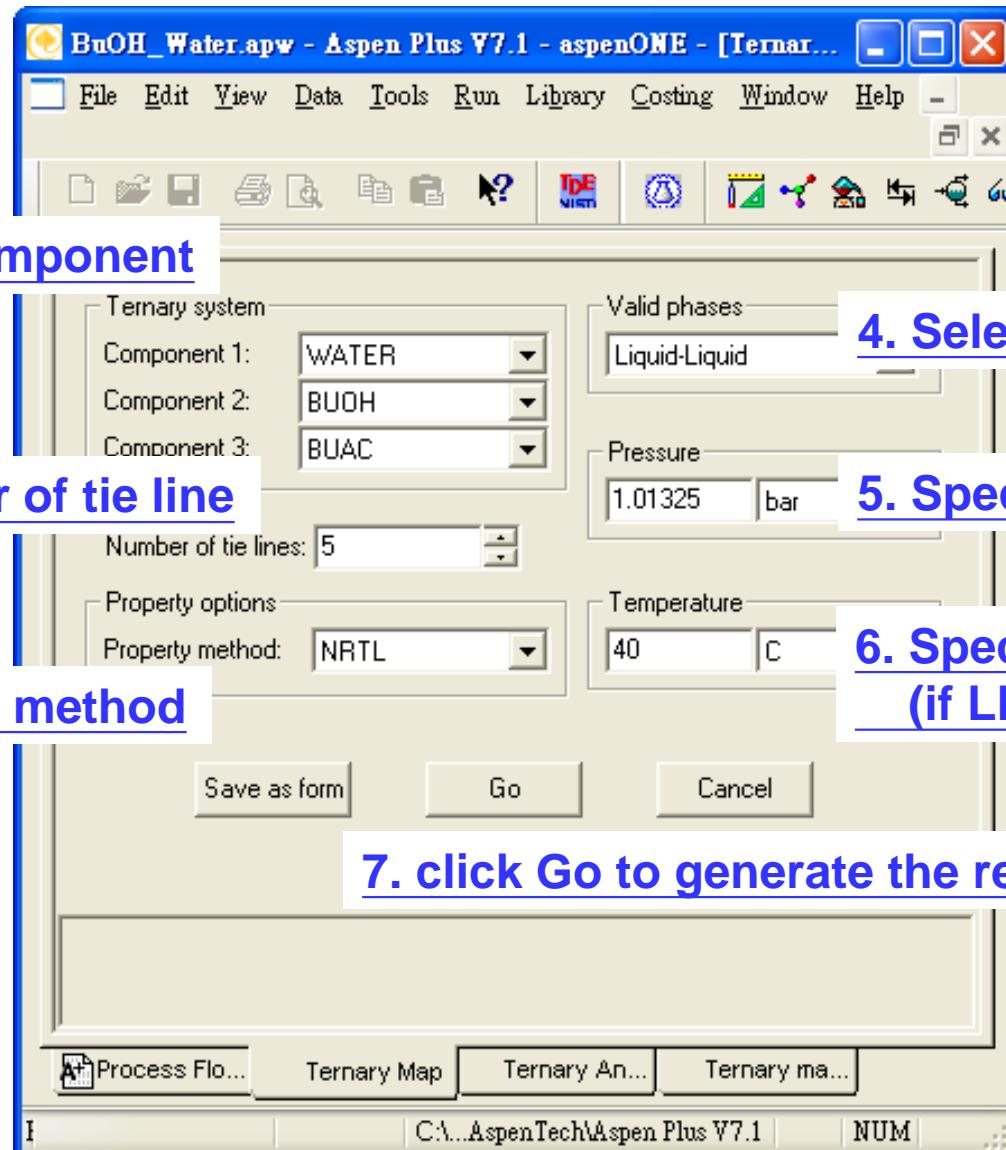
Component i	WATER	BUOH	BUAC
Component i	WATER	BUOH	BUAC
Temperature units	F	F	F
Source	APV72 VLE-IG	APV72 VLE-IG	APV72 VLE-IG
Property units:			
AJJ	13.11020000	5.023900000	1.760900000
AJI	-2.040500000	-1.513200000	-3.029600000
BIJ	-6010.116432	510.7809559	-773.3507338
BJI	1374.964549	1792.746886	2019.849284

Text Overlay: "3 components -> 3 set of binary parameter (How about 4 components??)"

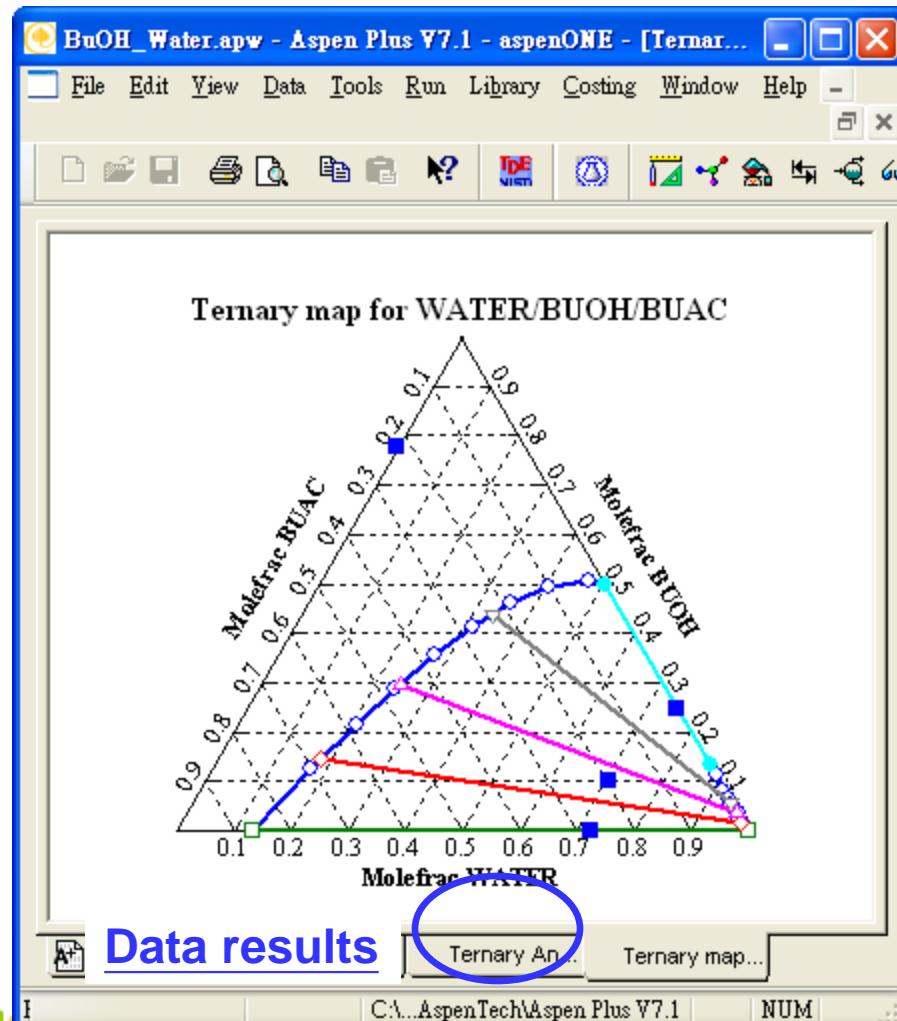
Properties Analysis – Ternary



Ternary Map



Calculation Result of Ternary Map (LLE)



Select results

Phase envelope Equilibrium compositions Azeotrope

Phase envelope compositions

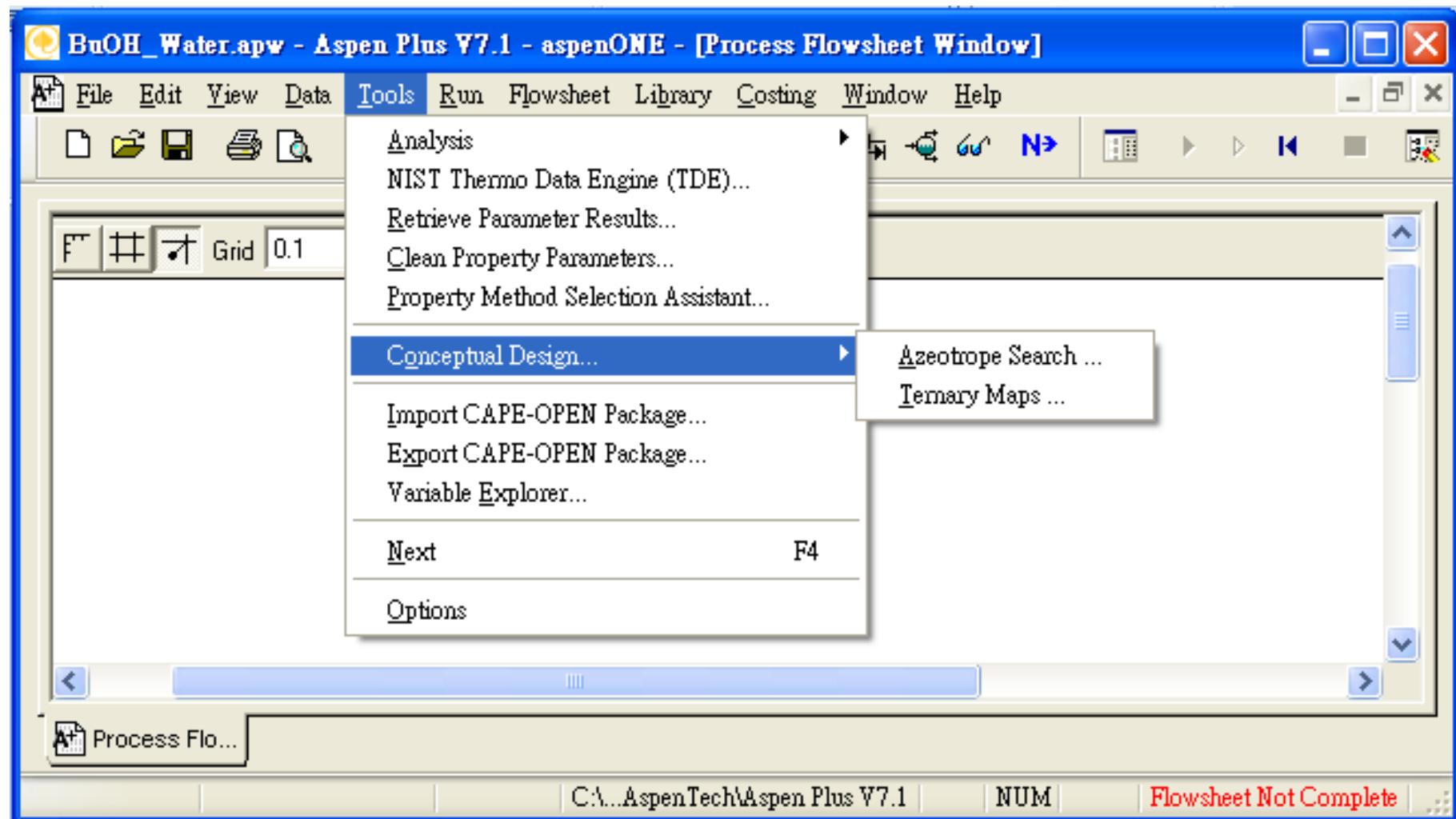
NUMBER	MOLEFRAC WATER	MOLEFRAC BUOH	MOLEFRAC BUAC
1	0.1339997	0	0.8660003
1	0.1758284	0.1274107	0.6967609
1	0.2089015	0.2135126	0.5775859
1	0.2423057	0.2890252	0.468669
1	0.2768588	0.3552938	0.3678474
1	0.3137713	0.4125953	0.2736334
1	0.3549945	0.4599584	0.1850471
1	0.4039997	0.49401	0.1019903
1	0.4683113	0.5052494	0.0264392
1	0.502051	0.497949	0
1	0.8661294	0.1338706	0
1	0.886776	0.1117443	0.00147973
1	0.9168318	0.0806885	0.00247966
1	0.933726	0.0637595	0.00251452
1	0.9454354	0.0522048	0.00235979
1	0.9549068	0.0429395	0.0021537

Property Analysis – Conceptual Design

(Optional)

Use this form	To generate
Pure	Tables and plots of pure component properties as a function of temperature and pressure
Binary	Txy, Pxy, or Gibbs energy of mixing curves for a binary system
Residue	Residue curve maps
Ternary	Ternary maps showing phase envelope, tie lines, and azeotropes of ternary systems
Azeotrope	This feature locates all the azeotropes that exist among a specified set of components.
Ternary Maps	Ternary diagrams in Aspen Distillation Synthesis feature: Azeotropes, Distillation boundary, Residue curves or distillation curves, Isovatility curves, Tie lines, Vapor curve, Boiling point

Conceptual Design



Azeotrope Analysis

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Analysis
NIST Thermo Data Engine (TDE)...
Retrieve Parameter Results...
Clean Property Parameters...
Property Method Selection Assistant...
Conceptual Design... *Azeotrope Search ...* *Ternary Maps ...*
Import CAPE-OPEN Package...
Export CAPE-OPEN Package...
Variable Explorer...
Next F4
Options

Setup
Components
Properties
Flowsheet
Streams
Blocks
Utilities
Reactions
Convergence
Flowsheeting O:
Model Analysis Tools
EO Configuration
Results Summary
Dynamic Configuration

Process Flo... Data Browser

Search Azeotropes C:\...\AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

Green Chemical Process Technology aspentech process. to the power of a.

Azeotrope Analysis

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Azeotrope Analysis]

File Edit View Data Tools Run Library Costing Window Help

1. Select components (at least two)

Component List

Name	Description
WATER	WATER
BUOH	N-BUTANOL
BUAC	N-BUTYL-ACETATE

2. Specify pressure

Pressure: 101325 N/SQM

3. Select property method

Model: NRTL

Phases: VAP-LIQ

4. Select phase (VLE, LLE)

Report Units

Temperature: C

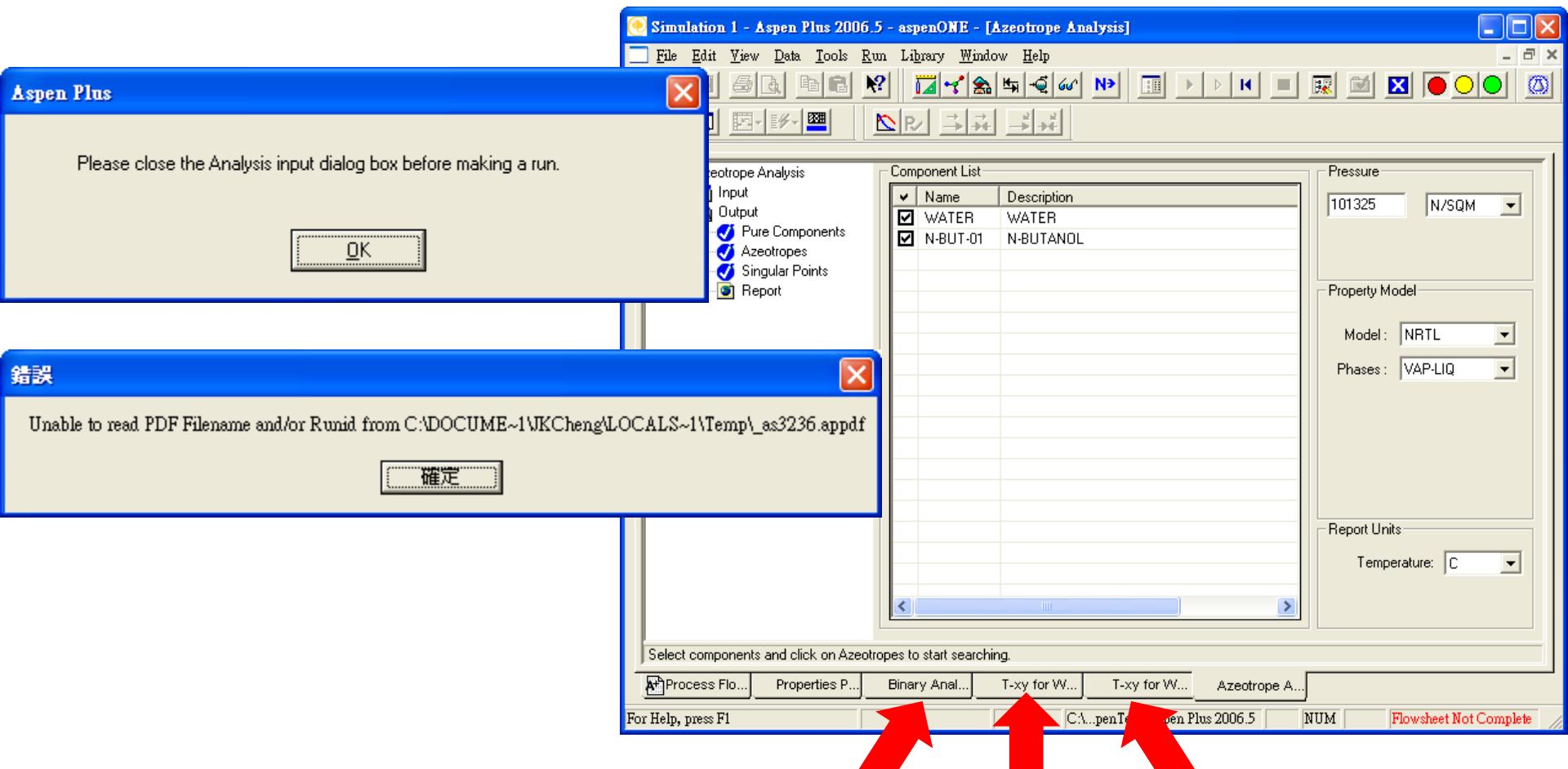
5. Select report Unit

Select components and click on Azeotropes to start searching.

Process Flo... Data Bro... Azeotrope A...

For Help, press F1 | C:\...AspenTech\Aspen Plus V7.1 | NUM | Flowsheet Not Complete |

Error Message



Close analysis input dialog box (pure or binary analysis)

Azeotrope Analysis Report

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Azeotrope Analysis]

File Edit View Data Tools Run Library Costing Window Help

Azeotrope Analysis

- Input
- Output
 - Pure Components
 - Azeotropes
 - Singular Points
 - Report

ASPEN SPLIT ANALYSIS

AZEOTROPE SEARCH REPORT

Physical Property Model: NRTL Valid Phase: VAP-LIQ-LIQ

Mixture Investigated For Azeotropes At A Pressure Of 101325 N/SQM

Comp ID	Component Name	Classification	Temperature
WATER	WATER	Stable Node	100.02 C
BUOH	N-BUTANOL	Stable Node	117.75 C
BUAC	N-BUTYL-ACETATE	Stable Node	126.01 C

4 Azeotropes Sorted by Temperature

01	Number Of Components: 2 Heterogeneous	Temperature 92.64 C	
		MOLE BASIS	MASS BASIS
WATER	0.7532	0.4258	
BUOH	0.2468	0.5742	

Idle

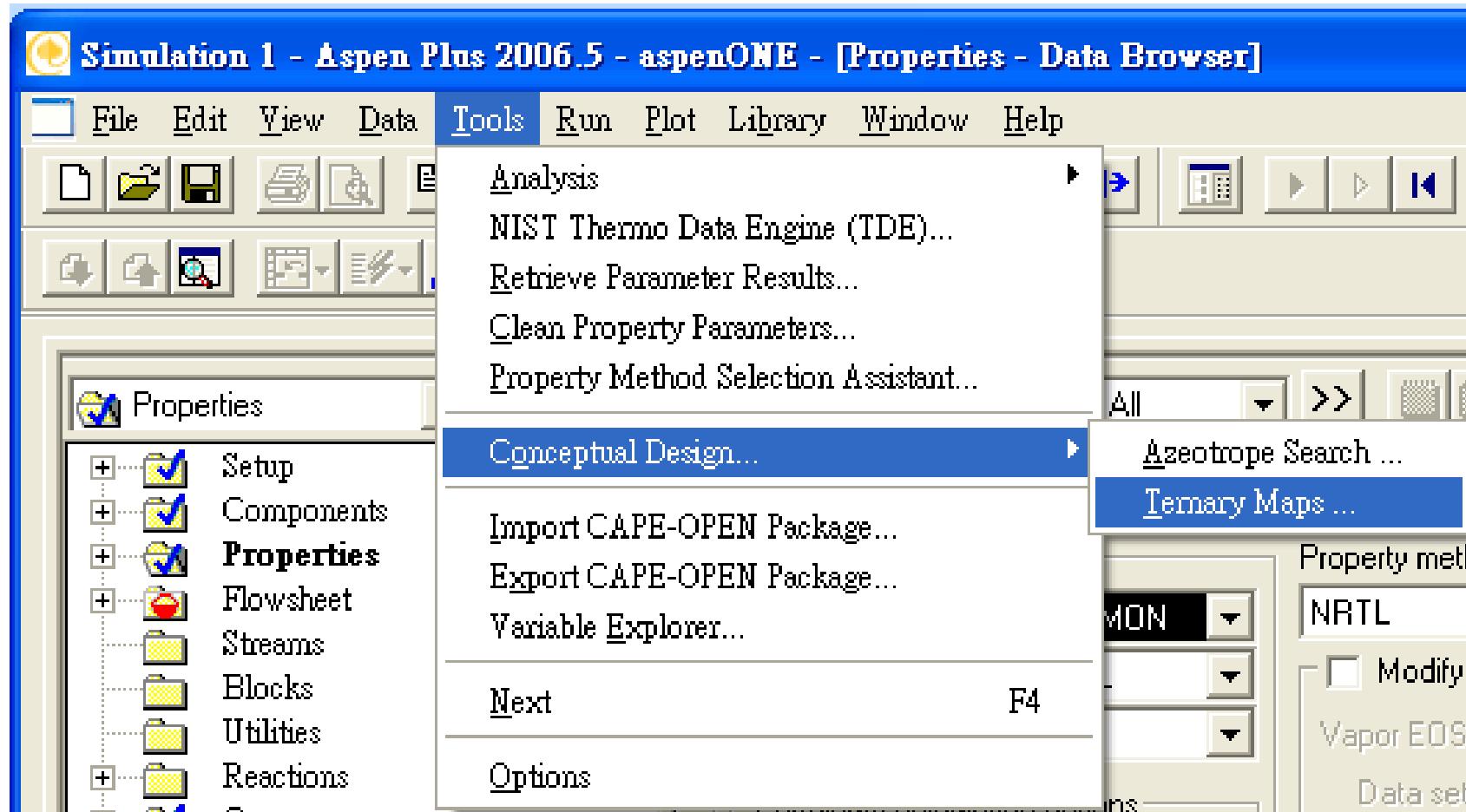
Process Flow... Azeotrope A...

C:\...AspenTech\Aspen Plus V7.1 NUM Flowsheet Not Complete

Green Chemical Process Technology

enTech

Ternary Maps



Ternary Maps

1. Select three components

2. Specify pressure

3. Select property method

4. Select phase (VLE, LLE)

5. Select report Unit

6. Click Ternary Plot to generate the results

**6. Specify temperature of LLE
(If liquid-liquid envelope is selected)**

File Edit View Data Tools Run Library Costing Window Help

Explorer Plot Input

TernaryMap Analysis

Input

Output

Pure Components

Azeotropes

Singular Points

Report

Ternary Plot

Comp 1 WATER

Comp 2 BUOH

Comp 3 BUAC

Pres 101325 N/SQM

VLE Model: NRTL

LLE Model: NRTL

Phases : VAP-LIQ

Basis

Mass Fraction

Mole Fraction

Temp Units

C

Distillation curve

Azeotropes

Distillation Boundary

Vapor-Liquid-Liquid Envelope

Liquid-Liquid Envelope

40 C

Isovatility curve

Click on Ternary Plot to generate the ternary map

Process Flow Data Browser Ternary Maps

For Help, press F1

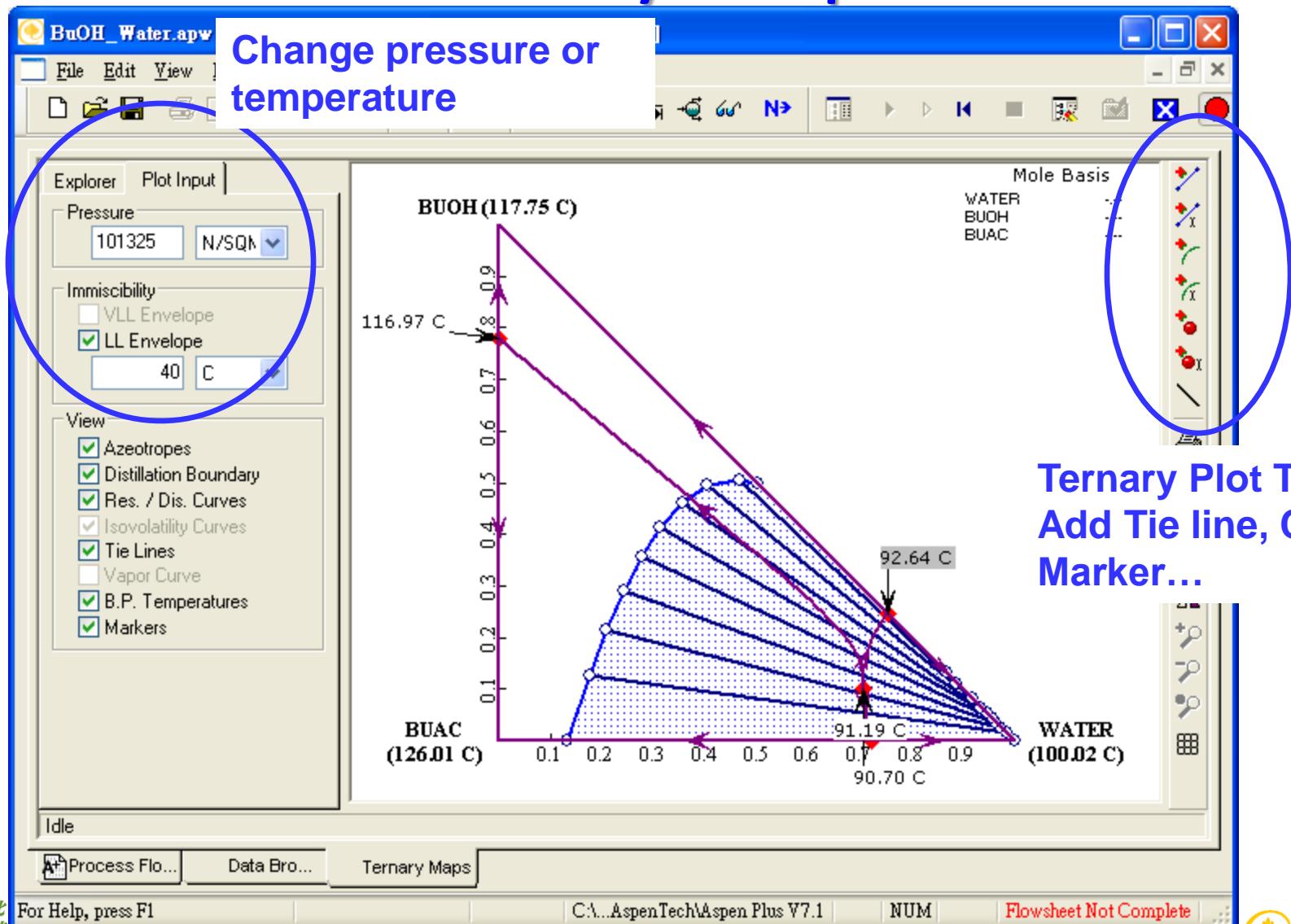
C:\...AspenTech\Aspen Plus V7.1

NUM

Flowsheet Not Complete

aspen tech

Ternary Maps



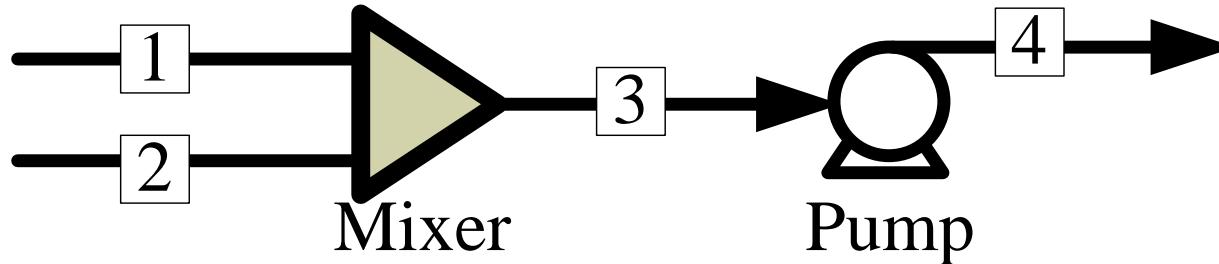
Introduction to Aspen Plus

Part 4: Running simulation

Simple Units

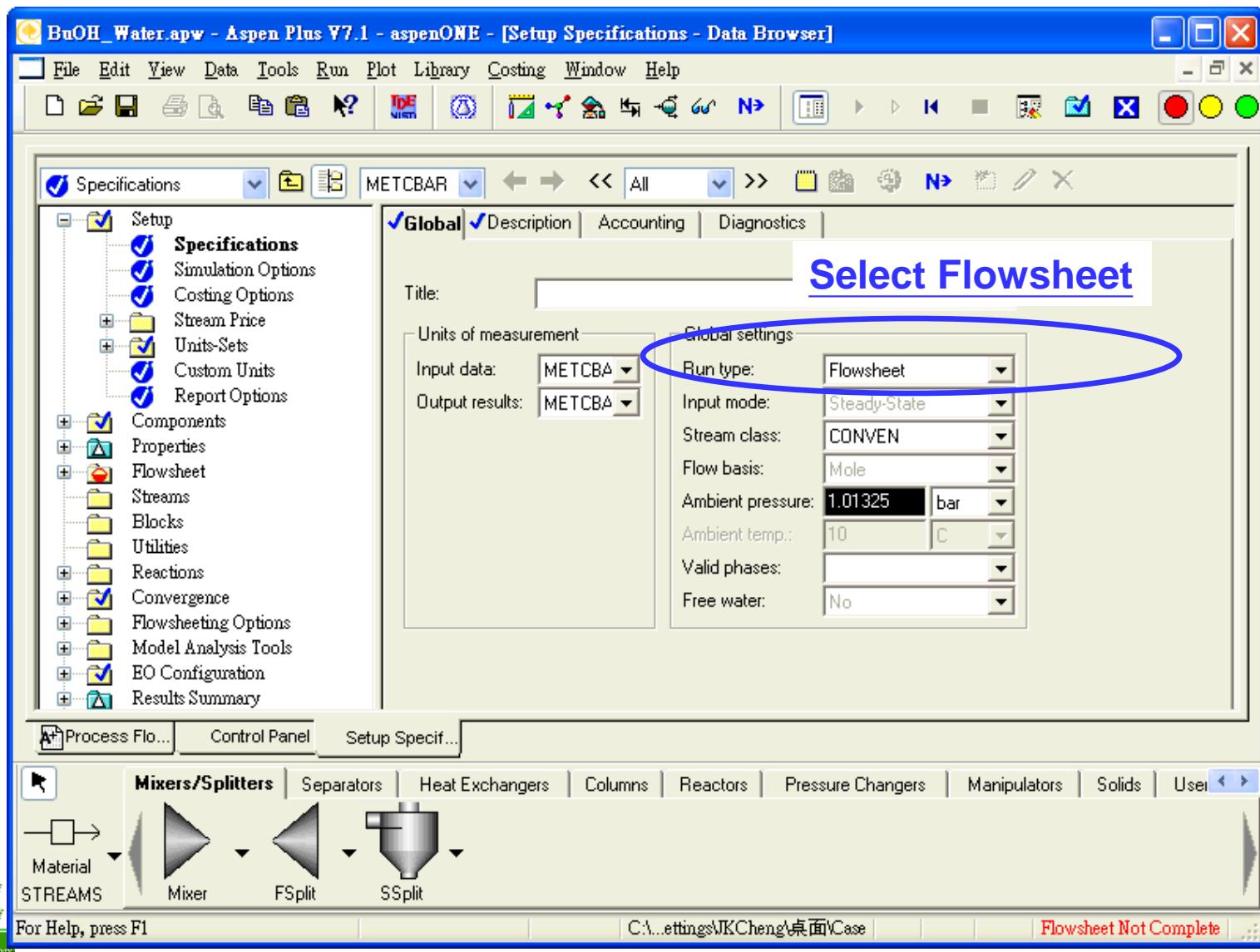
(Mixer, Pump, valve, flash, heat exchanger)

Example 1: Calculate the mixing properties of two stream

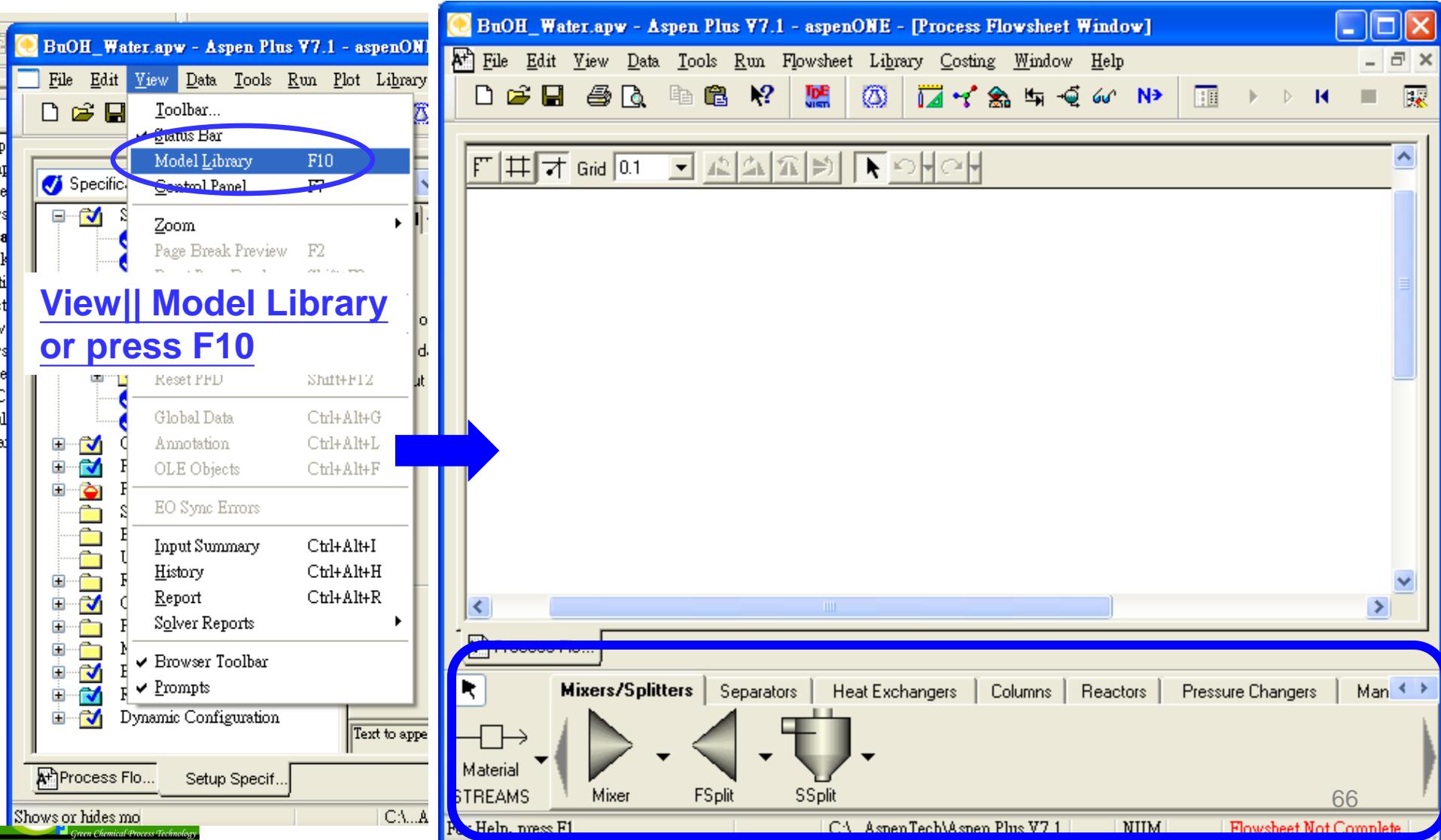


	1	2	3	4
Mole Flow kmol/hr				
WATER	10	0	?	?
BUOH	0	9	?	?
BUAC	0	6	?	?
Total Flow kmol/hr	10	15	?	?
Temperature C	50	80	?	?
Pressure bar	1	1	1	10
Enthalpy kcal/mol	?	?	?	?
Entropy cal/mol-K	?	?	?	?
Density kmol/cum	?	?	?	?

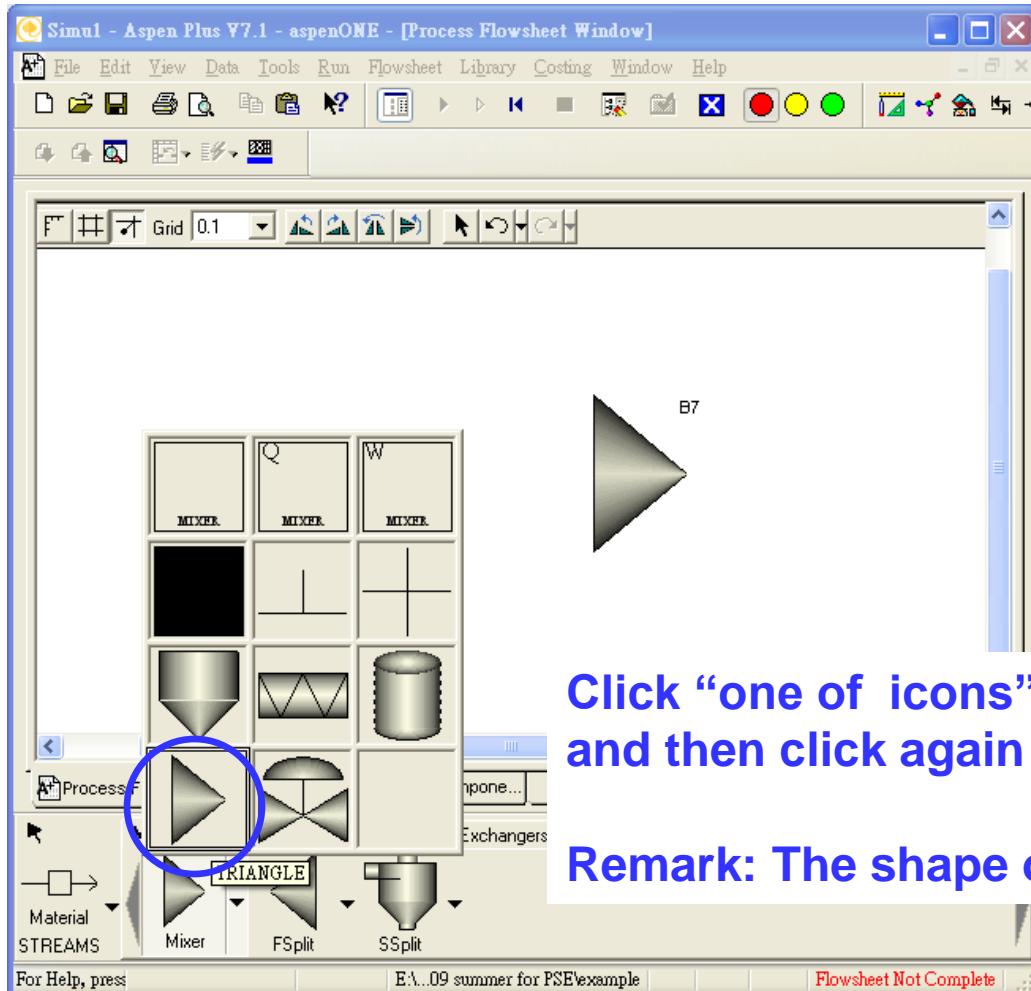
Setup – Specification



Reveal Model Library



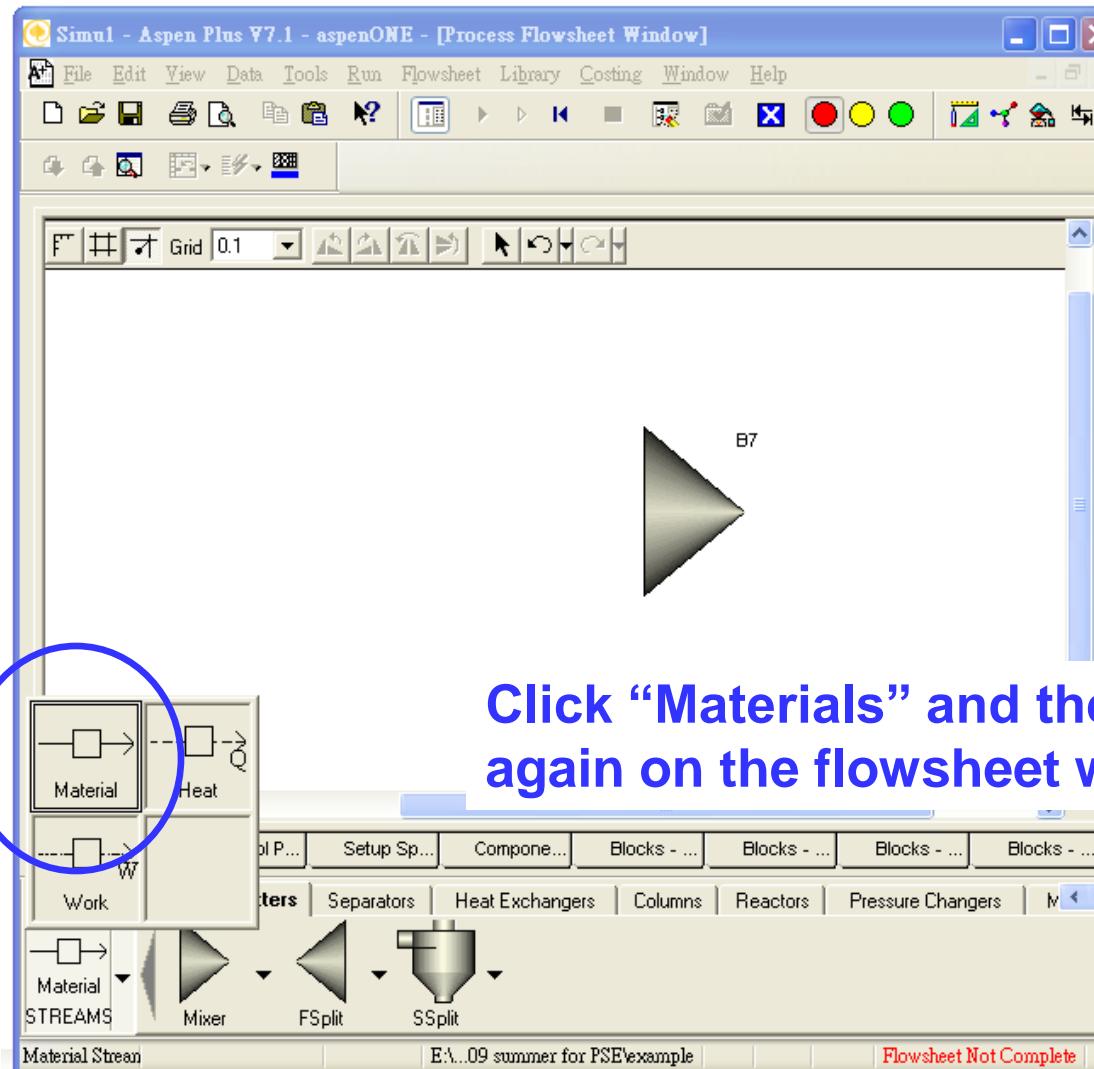
Adding a Mixer



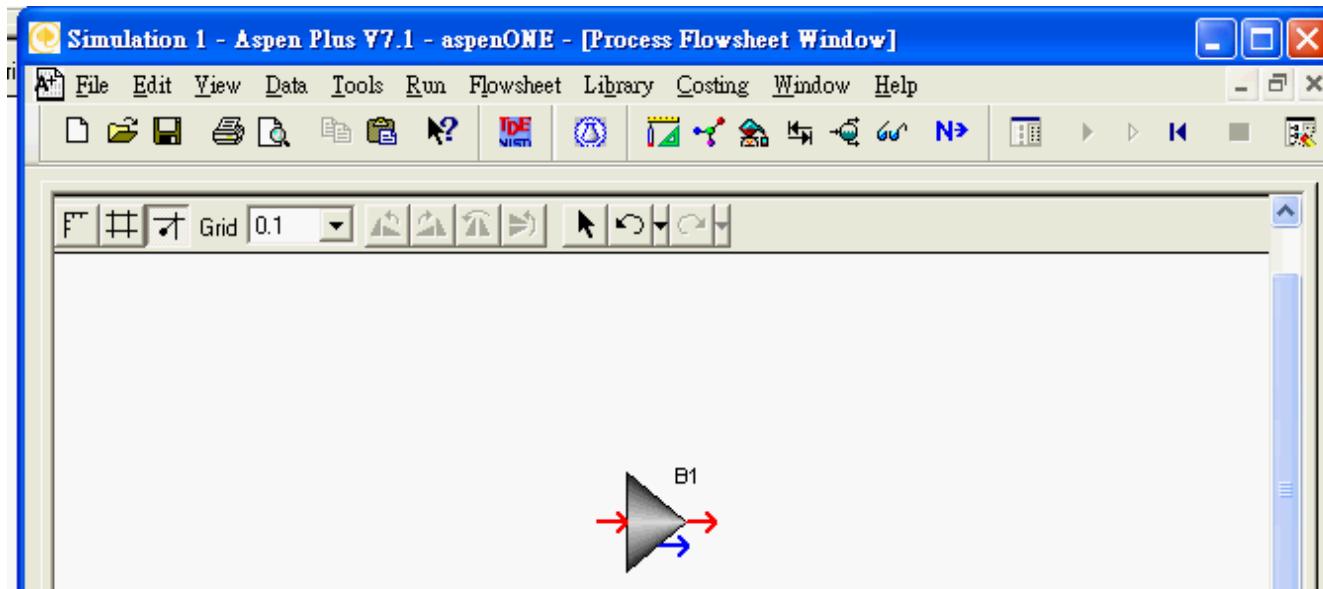
Click “one of icons”
and then click again on the flowsheet window

Remark: The shape of the icons are meaningless

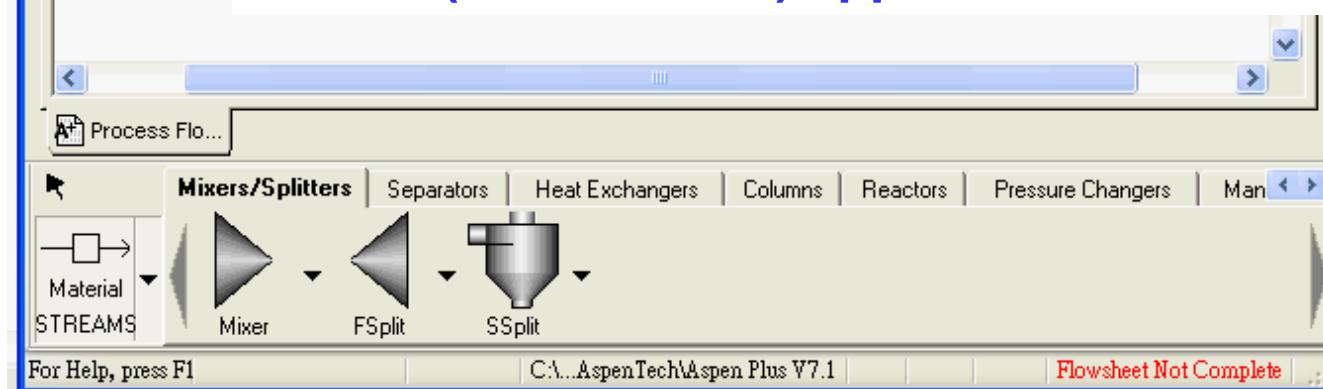
Adding Material Streams



Adding Material Streams (cont'd)

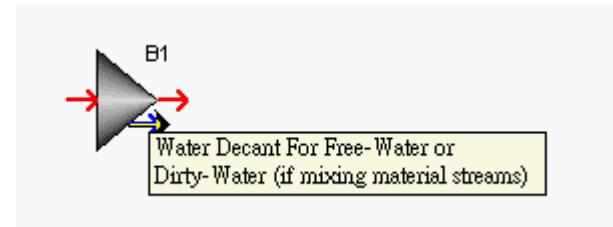
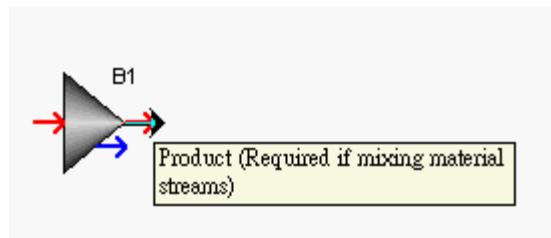
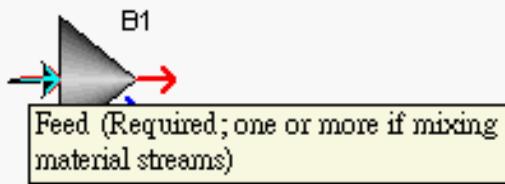


When clicking the mouse on the flowsheet window, arrows (blue and red) appear.



Adding Material Streams (cont'd)

When moving the mouse on the arrows, some description appears.

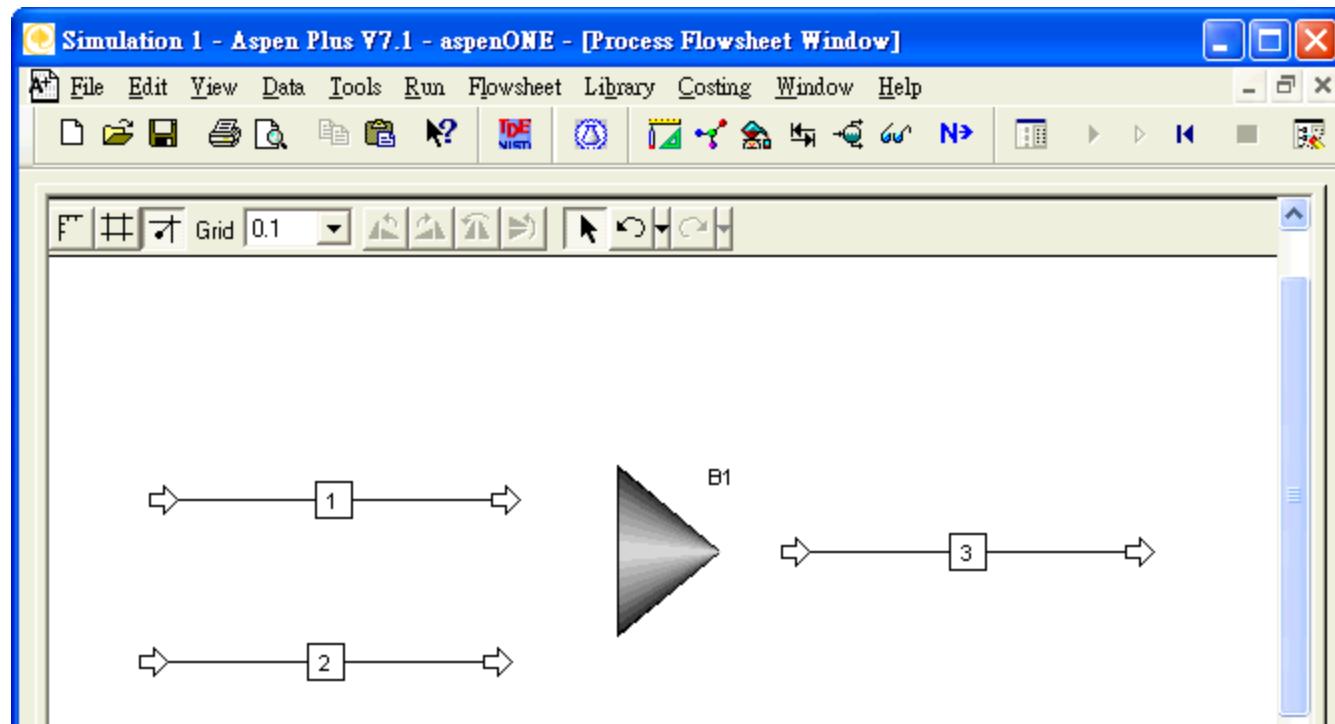


**Red arrow(Left) Feed
(Required; one ore more
if mixing material
streams)**

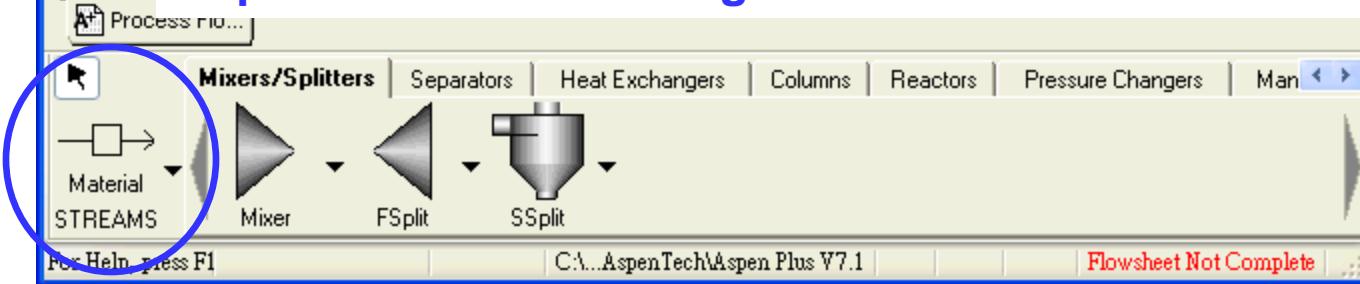
**Red arrow(Right):
Product (Required; if
mixing material streams)**

**Blue arrow: Water
decant for Free water
of dirty water.**

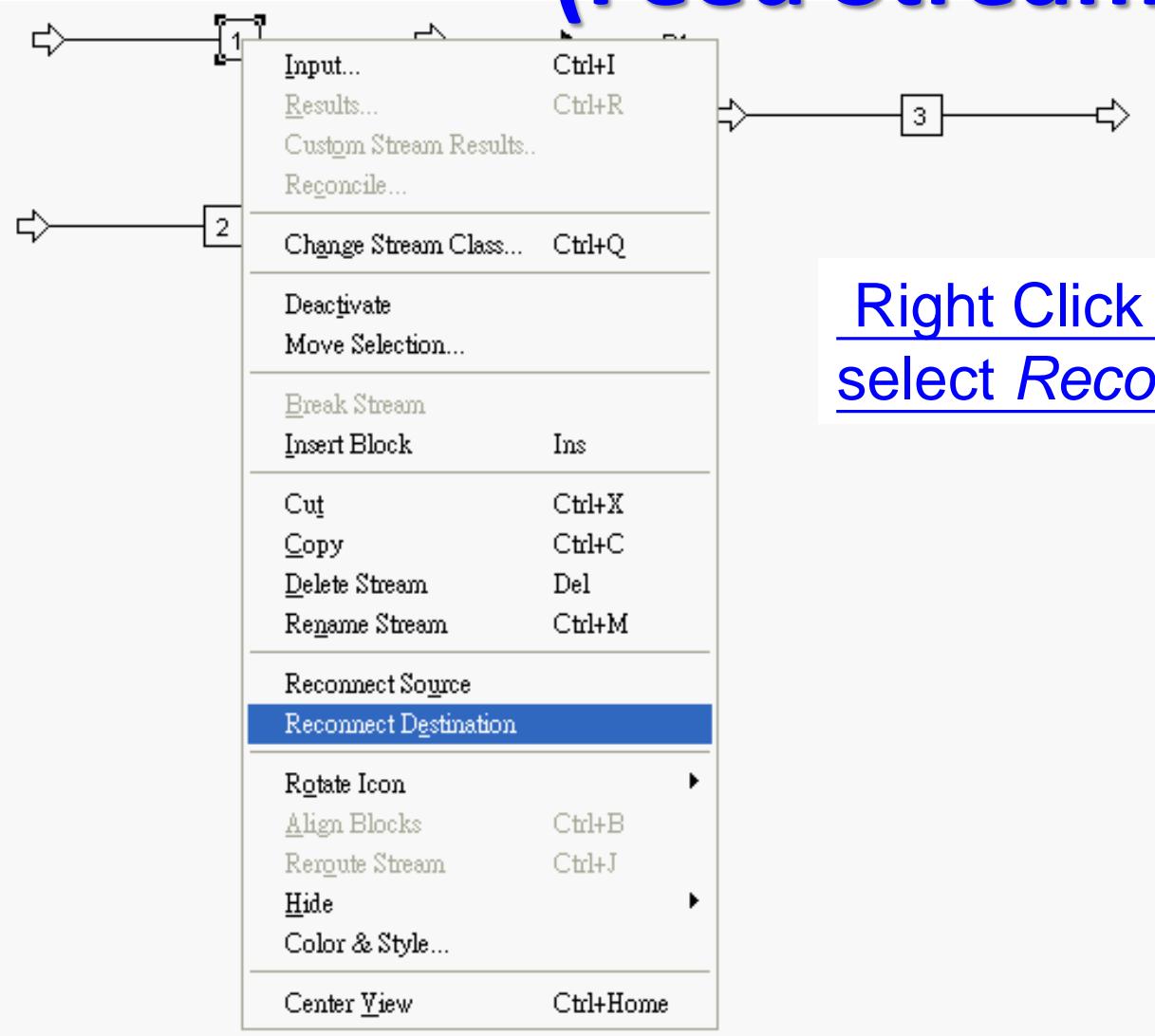
Adding Material Streams (cont'd)



After selecting “Material Streams”, click and pull a stream line.
Repeat it three times to generate three stream lines.

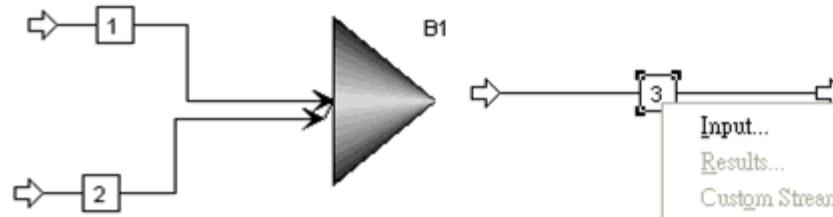


Reconnecting Material Streams (Feed Stream)



Right Click on the stream and
select *Reconnect Destination*

Reconnecting Material Streams (Product Stream)



Input... Ctrl+I

Results... Ctrl+R

Custom Stream Results...

Reconcile...

Change Stream Class... Ctrl+Q

Deactivate

Move Selection...

Break Stream

Insert Block Ins

Cut Ctrl+X

Copy Ctrl+C

Delete Stream Del

Rename Stream Ctrl+M

Reconnect Source

Reconnect Destination

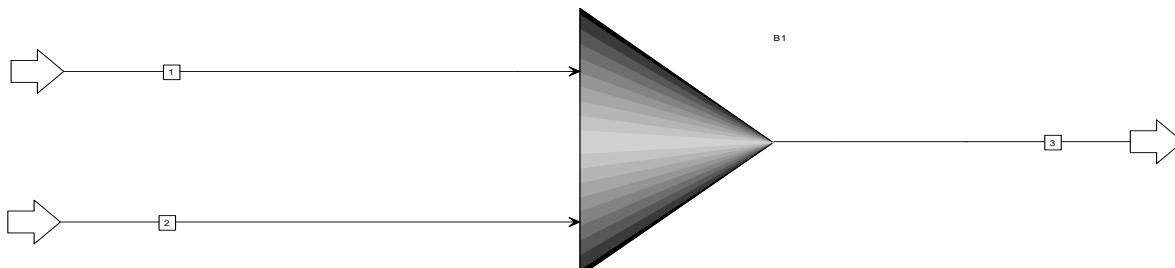
Rotate Icon

Align Blocks Ctrl+B

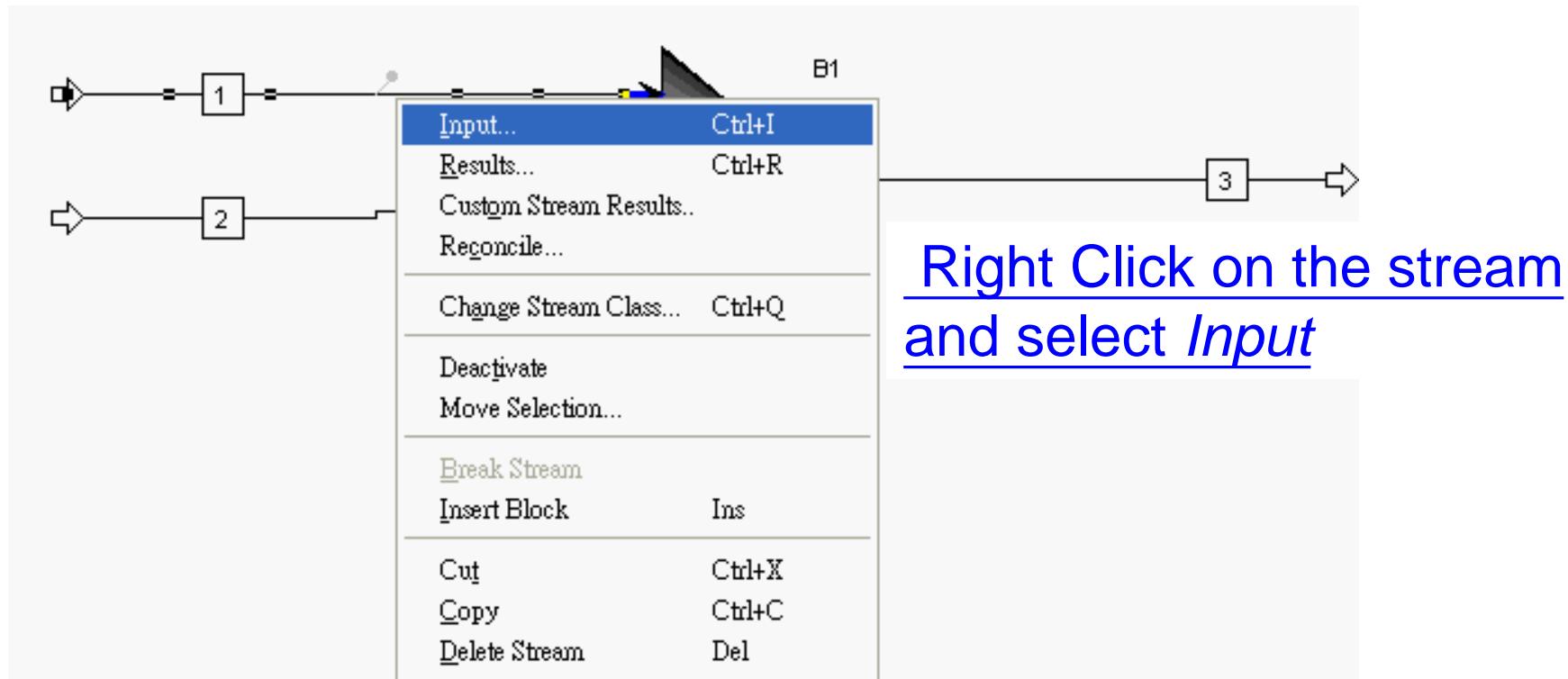
Reroute Stream Ctrl+J

Hide

Color & Style...



Specifying Feed Condition



Specifying Feed Condition (cont'd)

1

Specifications Flash Options PSD Component Attr. EO Option

Substream name: **MIXED** Ref Temperature

State variables

Temperature	50	C
Pressure	1	bar

Composition

Mole-Flow	kmol/hr
Component	Value
WATER	10
BUOH	
BUAC	

Total flow: Mole kmol/hr

Solvent:

2

Specifications Flash Options PSD Component Attr. EO Option

Substream name: **MIXED** Ref Temperature

State variables

Temperature	80	C
Pressure	1	bar

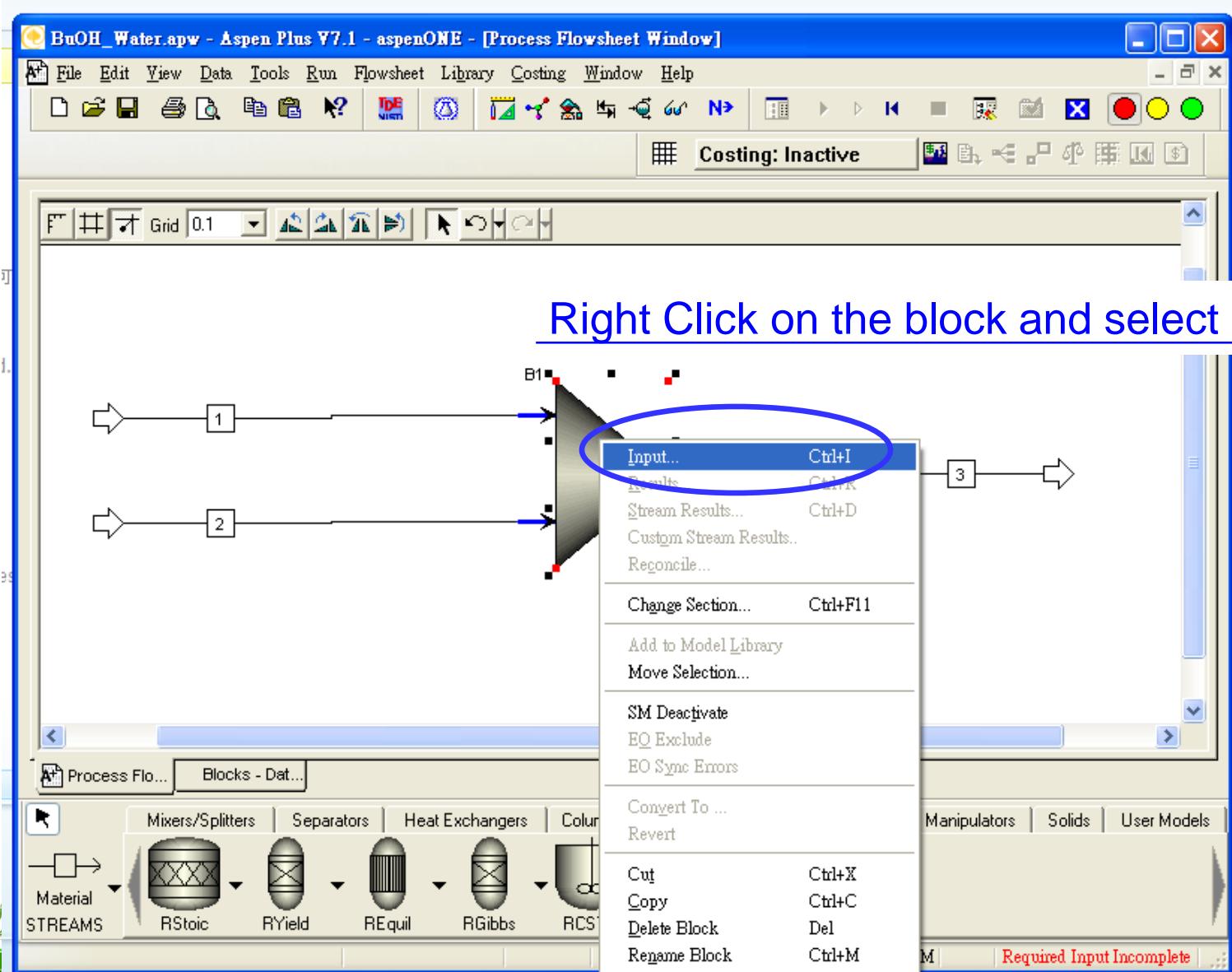
Composition

Mole-Frac	Component	Value
	WATER	
	BUOH	0.6
	BUAC	0.4

Total flow: Mole kmol/hr

Solvent:

Specifying Input of Mixer



Specifying Input of Mixer (cont'd)

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Block B1 (Mixer) - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Costing: Inactive

B1 Flash Options Mixer specifications

Pressure: 0 bar

Valid phases: Vapor-Liquid

Specify Pressure and valid phase

Temperature estimate: C

Convergence parameters

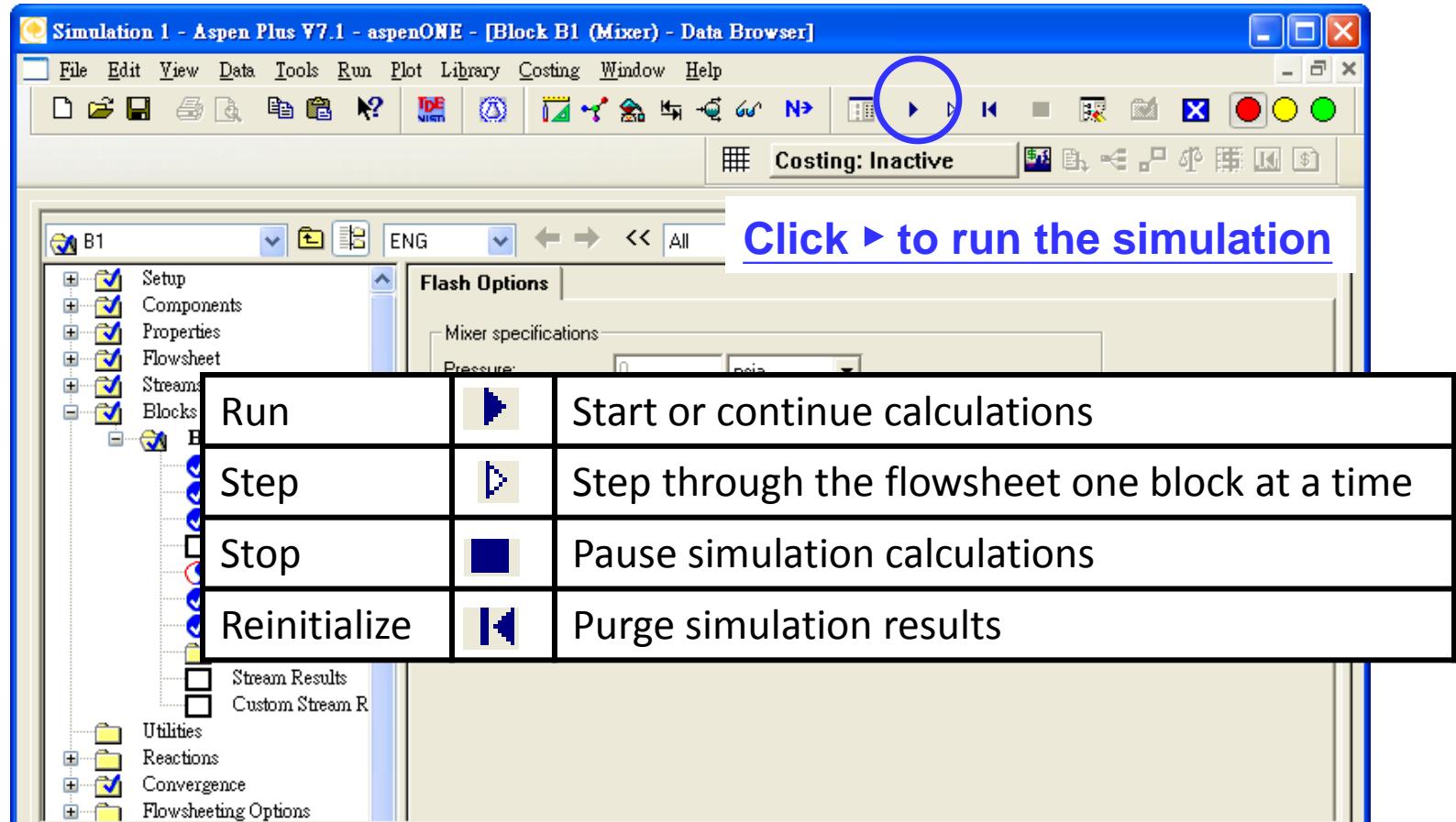
Maximum iterations: 30

Error tolerance: 0.0001

Let you type the pressure. Absolute units: Outlet pressure if value > 0; Pressure drop if value <= 0. Gauge units: Outlet pressure for all values.

The screenshot shows the Aspen Plus Data Browser interface. The title bar indicates the file is 'BuOH_Water.apw'. The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. A toolbar with various icons is visible above the main window. The main window has tabs for 'METCBAR' and 'All'. A status bar at the bottom says 'Costing: Inactive'. On the left, a tree view shows the project structure: 'B1' is expanded, showing 'Setup', 'Components', 'Properties', 'Flowsheet', 'Streams', and 'Blocks'. 'Blocks' is further expanded to show 'B1' with sub-options: 'Input', 'Dynamic', 'Block Options', 'Results', 'EO Variables', 'EO Input', 'Spec Groups', 'Ports', 'Stream Results', and 'Custom Stream R'. Below 'B1' are 'Utilities', 'Reactions', 'Convergence', 'Flowsheeting Options', 'Model Analysis Tools', 'EO Configuration', and 'Results Summary'. The central panel displays the 'Flash Options' dialog for 'Block B1 (Mixer)'. It has sections for 'Mixer specifications' (Pressure: 0 bar, Valid phases: Vapor-Liquid), 'Temperature estimate' (C), and 'Convergence parameters' (Maximum iterations: 30, Error tolerance: 0.0001). A blue annotation 'Specify Pressure and valid phase' is overlaid on the 'Pressure' field. At the bottom of the dialog, a note says 'Let you type the pressure. Absolute units: Outlet pressure if value > 0; Pressure drop if value <= 0. Gauge units: Outlet pressure for all values.' A small green logo is in the bottom left corner.

Run Simulation



Check “simulation status”

“Required Input Complete” means the input is ready to run simulation

Status of Simulation Results

The screenshot shows the Aspen Plus V7.1 Data Browser window. The title bar reads "BuOH_Water_Buac_Flowsheet - Aspen Plus V7.1 - aspenONE - [Block B1 (Mixer) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains icons for file operations like Open, Save, and Print, along with a search icon. The main area features a table with four columns: a sidebar with a tree view of the process flow sheet, a "Message" column, a "Means" column, and a "Details" column.

Message	Means
Results available	The run has completed normally, and results are present.
Results with warnings	Results for the run are present. Warning messages were generated during the calculations. View the Control Panel or History for messages.
Results with errors	Results for the run are present. Error messages were generated during the calculations. View the Control Panel or History for messages.
Input Changed	Results for the run are present, but you have changed the input since the results were generated. The results may be inconsistent with the current input.

A blue oval highlights the "Results Available" status in the bottom right corner of the table. The bottom navigation bar includes "For Help, press F1", a path "C:\...ettings\JKCheng\桌面\Case", and a "Results Available" button with a checkmark icon. The footer also features the "Green Chemical Process Technology" logo and the "OpenTech" logo.

Stream Results

The screenshot shows a process flow diagram in Aspen Plus. Stream 1 enters from the left and splits into two parallel paths. Stream 2 enters from the left and joins Stream 1. Both streams converge at a junction point, which then leads to Stream 3 exiting to the right. A context menu is displayed over Stream 3, listing options: Input... (Ctrl+I), Results... (Ctrl+R), Stream Results... (Ctrl+D, currently selected), Custom Stream Results.., Reconcile..., Change Section... (Ctrl+F11), Add to Model Library, Move Selection..., and SM Deactivate.

	1	2	3
Temperature C	50.0	80.0	70.1
Pressure bar	1.000	1.000	1.000
Vapor Frac	0.000	0.000	0.000
Mole Flow kmol/hr	10.000	15.000	25.000
Mass Flow kg/hr	180.153	1364.066	1544.218
Volume Flow cum/hr	0.186	1.740	1.871
Enthalpy MMkcal/hr	-0.678	-1.416	-2.094
Mole Flow kmol/hr			
'WATER	10.000		10.000
► BUOH		9.000	9.000
BUAC		6.000	6.000

E) **Right Click on the block and select Stream Results**

Display: Streams Format: **FULL** Stream Table

	1	2	3
Substream: MIXED			
Mole Flow kmol/hr			
WATER	10.00000	0.0	10.00000
BUOH	0.0	9.000000	9.000000
BUAC	0.0	6.000000	6.000000
Total Flow kmol/hr	10.00000	15.00000	25.00000
Total Flow kg/hr	180.1528	1364.066	1544.218
Total Flow cum/hr	0.1858196	1.740210	1.870509
Temperature C	50.00000	80.00000	70.08758
Pressure bar	1.000000	1.000000	1.000000
Vapor Frac	0.0	0.0	0.0

Pull down the list and select
“Full” to show more properties
results.



Enthalpy and Entropy

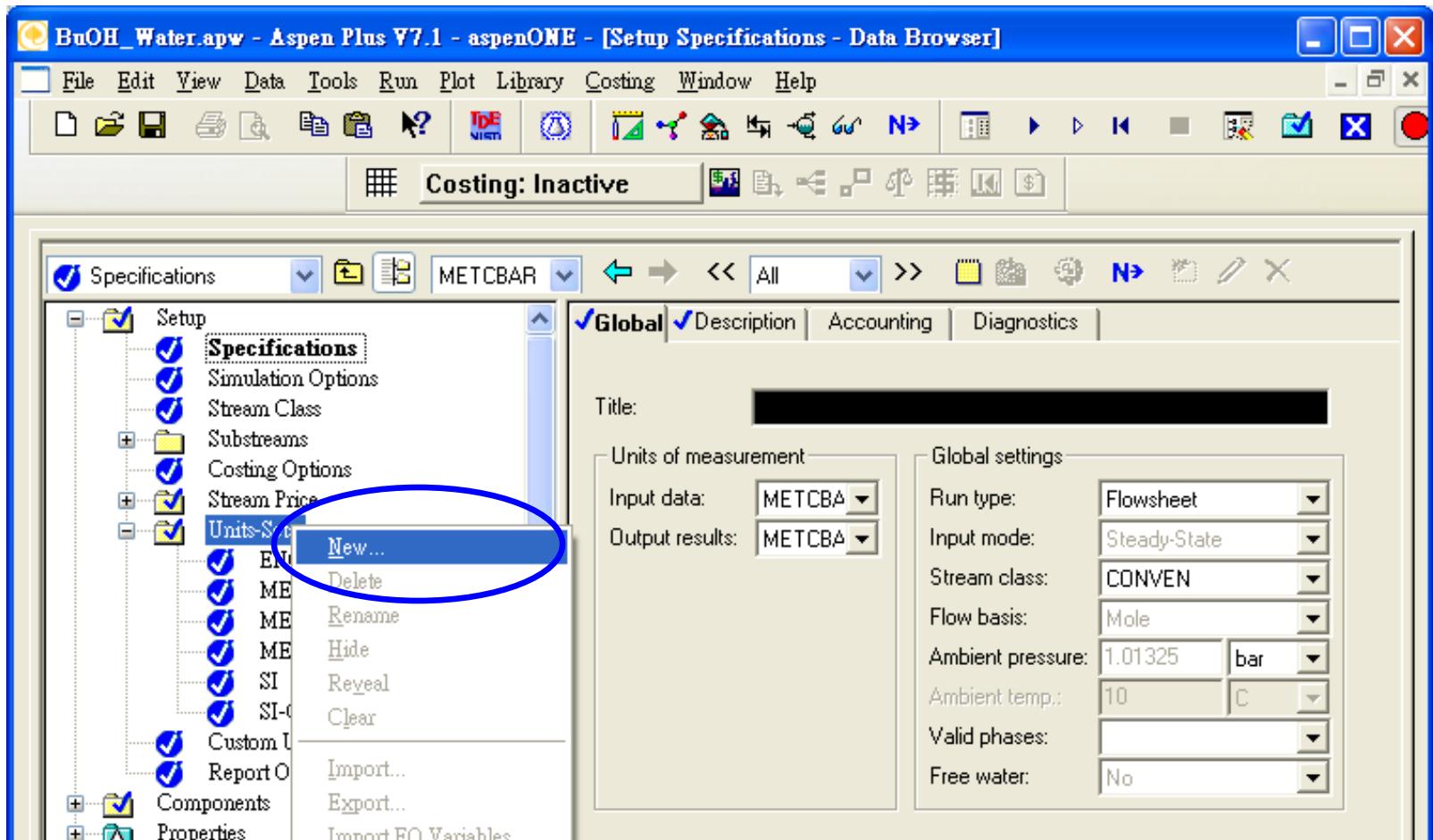
	1	2	3
Substream: MIXED			
Mole Flow kmol/hr			
WATER	10	0	10
BUOH	0	9	9
BUAC	0	6	6
Total Flow kmol/hr	10	15	25
Total Flow kg/hr	180.1528	1364.066	1544.218
Total Flow cum/hr	0.18582	1.74021	1.870509
Temperature C	50	80	70.08758
Pressure bar	2	1	1
Vapor Frac	0	0	0
Liquid Frac	1	1	1
Solid Frac	0	0	0
Enthalpy kcal/mol	-67.81	-94.3726	-83.7476
Enthalpy kcal/kg	-3764.03	-1037.77	-1355.82
Enthalpy Gcal/hr	-0.6781	-1.41559	-2.09369
Entropy cal/mol-K	-37.5007	-134.947	-95.6176
Entropy cal/gm-K	-2.0816	-1.48395	-1.54799
Density kmol/cum	53.81564	8.619647	13.36534
Density kg/cum	969.5038	783.851	825.5604
Average MW	18.01528	90.93771	61.76874
I60F cum/hr	0.1805	1.617386	1.797886

Change Units of Calculation Results

The screenshot shows the Aspen Plus Data Browser interface. The title bar reads "BuOH_Water_Buac_Flowsheet - Aspen Plus V7.1 - aspenONE - [Block B1 (Mixer) Stream Results - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and data analysis. The main window displays the "Stream Results" panel. On the left, there is a tree view with checked items: Streams, Blocks, B1 (with Results, EO Variables, Stream Results, and Custom Stream Results), and Results Summary. In the center, a dropdown menu is open over the unit selection field, showing options: ENG, MET, METCBAR, METCKGCM, SI, and SI-CBAR. Below the dropdown is a table titled "Streams" with three columns labeled 1, 2, and 3. The table contains data for various streams and their properties.

	1	2	3
Substream: MIXED			
Mole Flow lbmol/hr			
WATER	22.04623	0.0	22.04623
BUOH	0.0	19.84160	19.84160
BUAC	0.0	13.22774	13.22774
Total Flow lbmol/hr	22.04623	33.06934	55.11557
Total Flow lb/hr	397.1690	3007.250	3404.419
Total Flow cft/hr	6.562157	61.45495	66.05642
Temperature F	122.0000	176.0000	158.1576
Pressure psia	14.50377	14.50377	14.50377
Vapor Frac	0.0	0.0	0.0

Setup – Defining Your Own Units Set



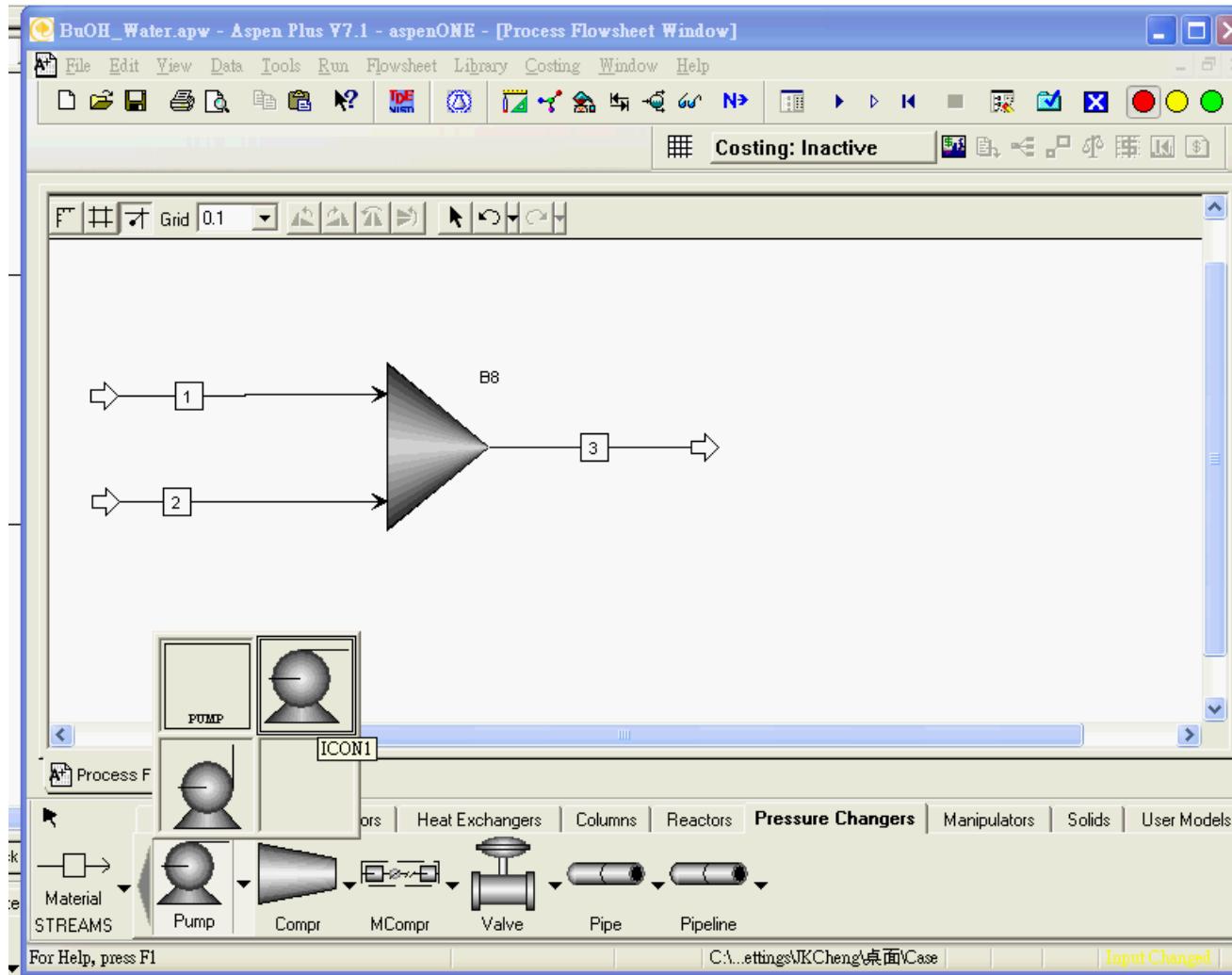
Setup – Report Options

The screenshot shows the Aspen Plus V7.1 interface with the title bar "BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Setup Report Options - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The main window has a tab bar with "Costing: Inactive" selected. On the left, a tree view under "Report Options" shows checked items: Setup, Specifications, Simulation Options, Stream Class, Substreams, Costing Options, Stream Price, Unit Sets, Custom Units, and Report Options. The "Report Options" item is circled in blue. The central panel has tabs for General, Flowsheet, Block, Stream (which is selected), Property, and ADA. Under Stream, there are sections for "Generate a standard stream report" (with checkboxes for "Include stream descriptions" and "Components with zero flow or fraction"), "Flow basis" (checkboxes for Mole, Mass, and Std.liq.volume), "Fraction basis" (checkboxes for Mole, Mass, and Std.liq.volume), "Stream format" (TFF: FULL dropdown, Standard (80 column) radio button selected, Wide (132 column) radio button, and Sort streams alphanumerically checkbox), and buttons for "Include Streams", "Exclude Streams", "Property Sets", and "Component Attributes". At the bottom, there are buttons for Stream Names, Batch Operation, and Supplementary Stream. The bottom navigation bar includes tabs for Process..., Results..., Stream..., Blocks..., and various block types like Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, and User. A toolbar below the navigation bar shows icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT.

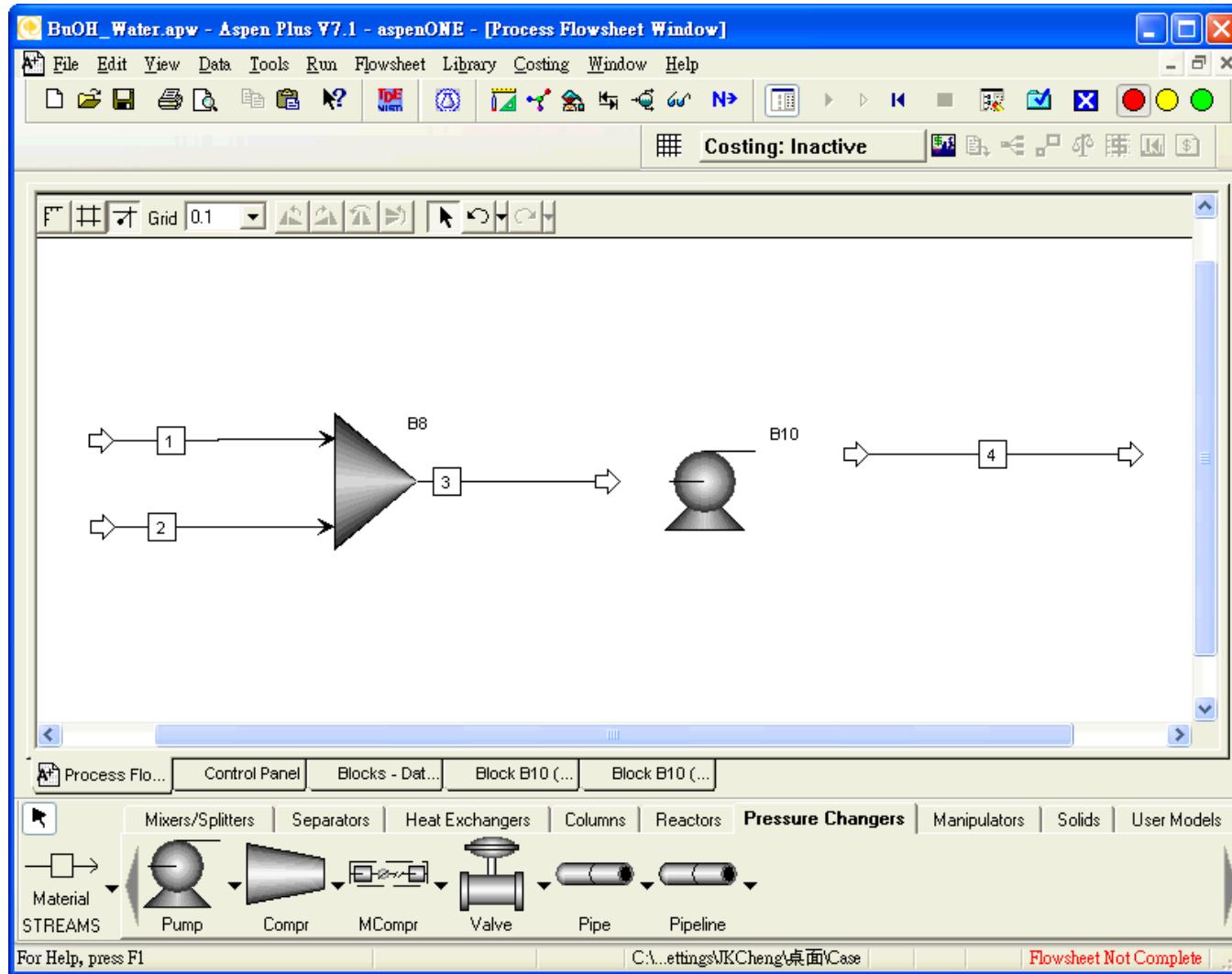
Stream Results with Format of Mole Fraction

Display:	Streams	Format:	FULL	Stream Table
	1	2	3	
Substream: MIXED				
Mole Flow kmol/hr				
WATER	10.00000	0.0	10.00000	
BUOH	0.0	9.000000	9.000000	
BUAC	0.0	6.000000	6.000000	
Mole Frac				
WATER	1.000000	0.0	.4000000	
BUOH	0.0	.6000000	.3600000	
BUAC	0.0	.4000000	.2400000	
Total Flow kmol/hr	10.00000	15.00000	25.00000	
Total Flow kg/hr	180.1528	1364.066	1544.218	

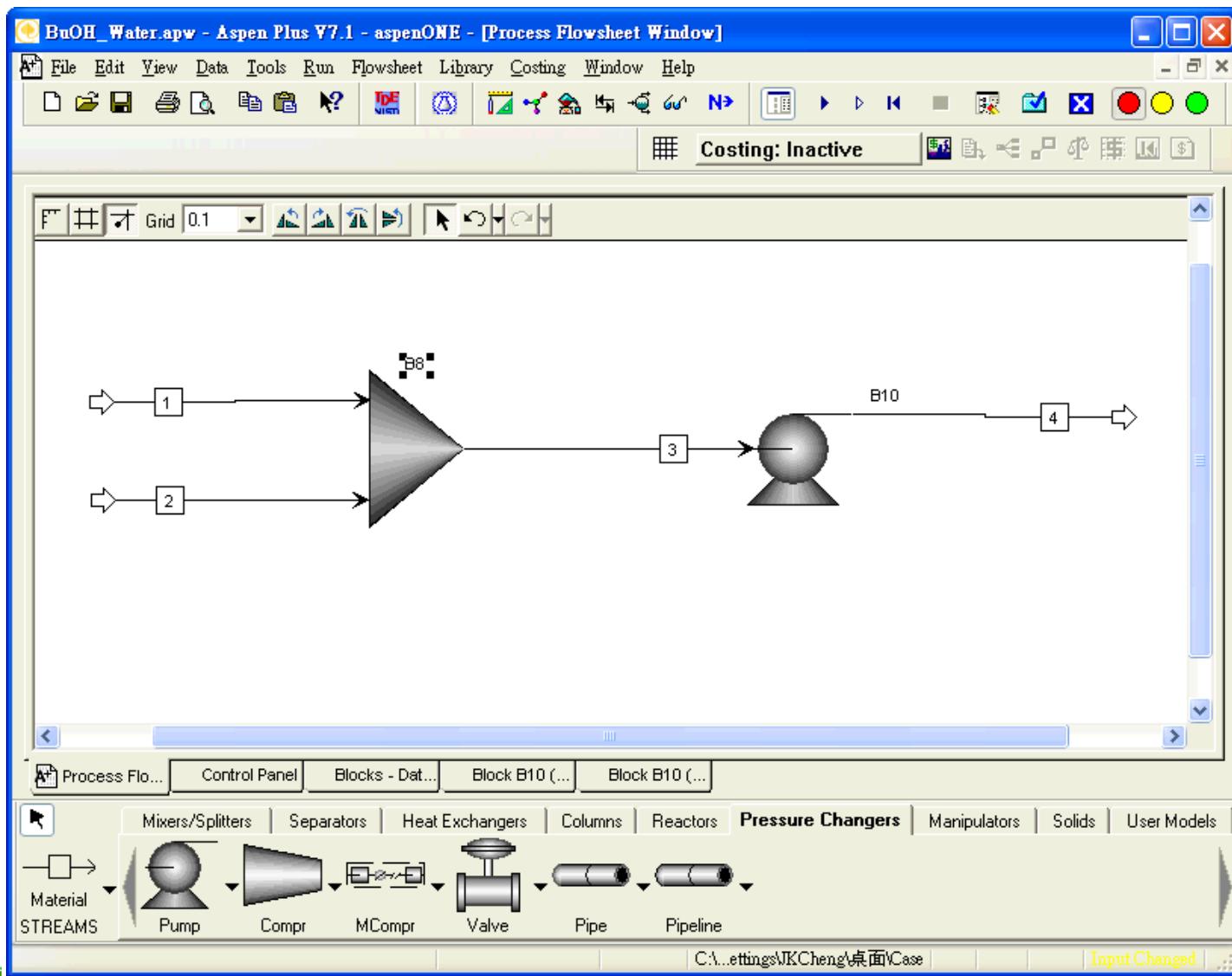
Add Pump Block



Add A Material Stream



Connect Streams



Pump – Specification

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Block B10 (Pump) - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Costing: Inactive

1. Select “Pump” or “turbine”

2. Specify pump outlet specification (pressure, power)

3. Efficiencies (Default: 1)

Model: Pump Turbine

Pump outlet specification:

- Discharge pressure: 10 bar
- Pressure increase:
- Pressure ratio:
- Power required:
- Use performance curve to determine discharge conditions

Efficiencies:

Pump: Driver:

Process Flow Control Panel Blocks - Dat... Block B10 (...) Block B10 (...) Block B10 (P...
Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models
Material STREAMS Pump Compr MCompr Valve Pipe Pipeline
For Help, press F1 C:\...ettings\JKCheng桌面\Case Input Changed

Run Simulation

BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Block B10 (Pump) Setup - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

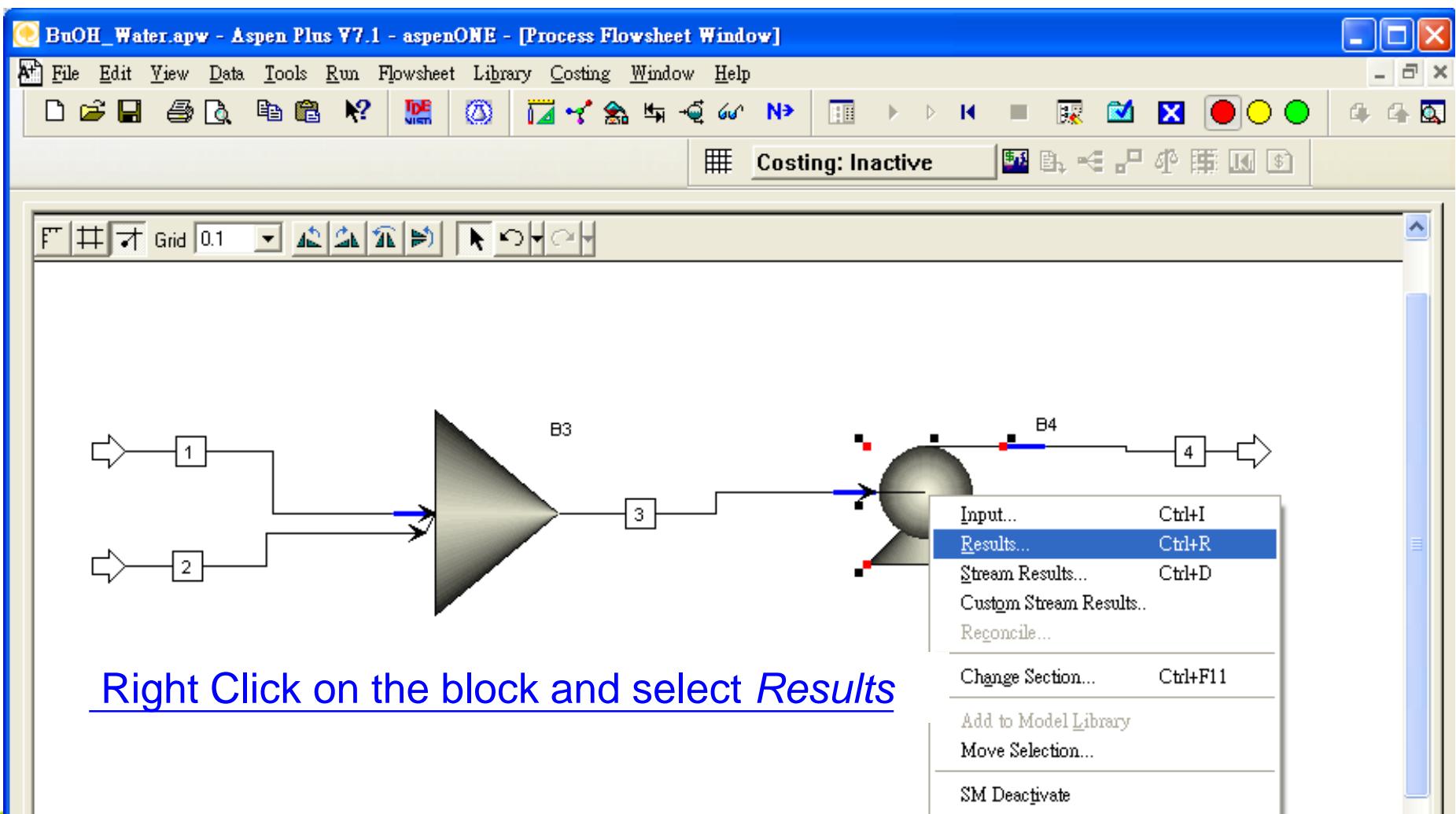
Costing: inactive

Click ► to generate the results

Check “simulation status”
“Required Input Complete”

The screenshot shows the Aspen Plus software interface. The title bar reads "BuOH_Water.apw - Aspen Plus V7.1 - aspenONE - [Block B10 (Pump) Setup - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons. A blue circle highlights the play button icon in the toolbar. The main window displays the "Setup" tab for "Block B10 (Pump) Setup". The left sidebar lists categories like Setup, Components, Properties, Flowsheet, Streams, and Blocks, with "B10" selected. The right panel shows the "Specifications" tab with options for Model (set to Pump), Pump outlet specification (discharge pressure set to 10 bar), Efficiencies, and other parameters. A large blue circle highlights the play button icon in the toolbar. Below the main window, a toolbar has a blue circle highlighting the "Input Changed" message. The bottom status bar shows "For Help, press F1" and a file path "C:\Settings\JKCheng\桌面\Case".

Block Results (Pump)





Costing: Inactive

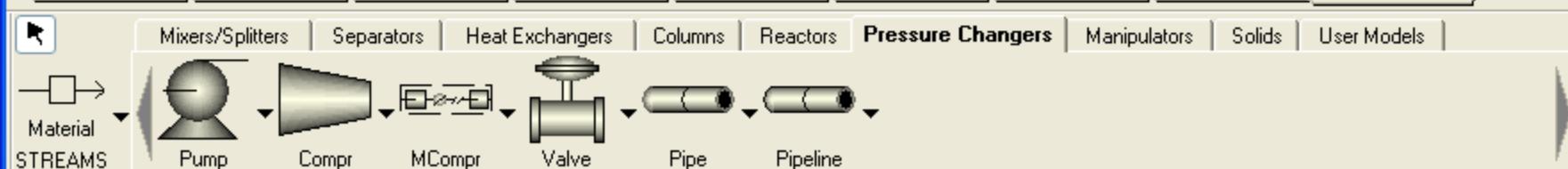
Results

- Streams
- Blocks
 - B3
 - B4
 - Results**
 - EO Variables
 - Stream Results
 - Custom Stream Resu...
- Results Summary

Summary Balance Performance Curve Utility Usage

Pump results

Fluid power:	0.46762735	kW
Brake power:	1.5816515	kW
Electricity:	1.5816515	kW
Volumetric flow rate:	1.87050937	cum/hr
Pressure change:	9	bar
NPSH available:	6.69862857	meter
NPSH required:		
Head developed:	111.166255	meter
Pump efficiency used:	0.29565764	
Net work required:	1.5816515	kW



Streams Results

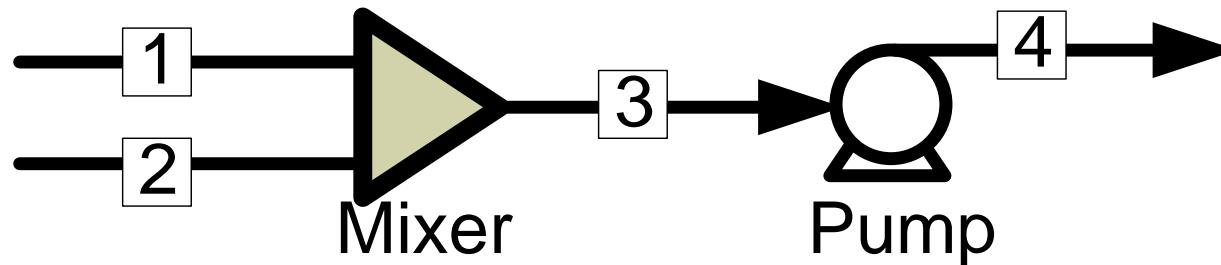
Display: Streams

Format: FULL

Stream Table

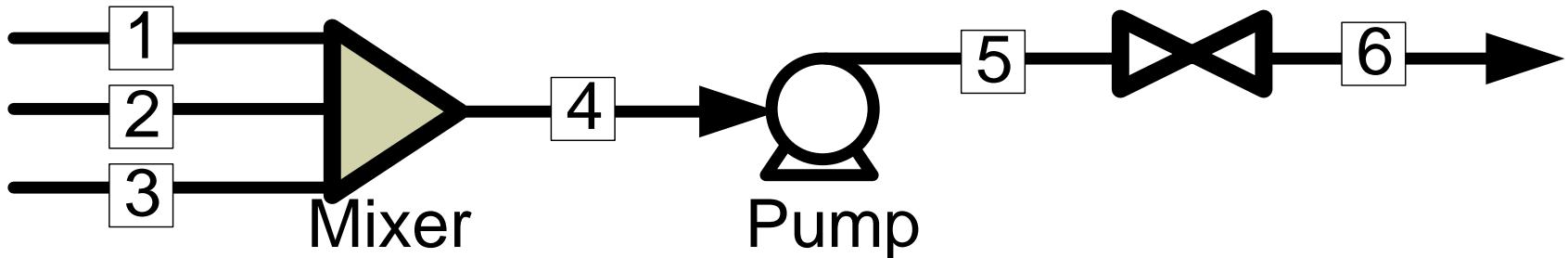
	1	2	3	4	
Total Flow kmol/hr	10.00000	15.00000	25.00000	25.00000	
Total Flow kg/hr	180.1528	1364.066	1544.218	1544.218	
Total Flow cum/hr	.1858196	1.740210	1.870509	1.873389	
Temperature C	50.00000	80.00000	70.08758	71.20504	
Pressure bar	1.000000	1.000000	1.000000	10.00000	
Vapor Frac	0.0	0.0	0.0	0.0	
Liquid Frac	1.000000	1.000000	1.000000	1.000000	
Solid Frac	0.0	0.0	0.0	0.0	
Enthalpy kcal/mol	-67.81001	-94.37261	-83.74757	-83.69317	
Enthalpy kcal/kg	-3764.028	-1037.772	-1355.824	-1354.944	
Enthalpy MMkcal/hr	-6781001	-1.415589	-2.093689	-2.092329	

Calculation Results (Mass and Energy Balances)



	1	2	3	4
Mole Flow kmol/hr				
WATER	10	0	10	10
BUOH	0	9	9	9
BUAC	0	6	6	6
Total Flow kmol/hr	10	15	25	25
Temperature C	50	80	70.09	71.20
Pressure bar	1	1	1	10
Enthalpy kcal/mol	-67.81	-94.37	-83.75	-83.69
Entropy cal/mol-K	-37.50	-134.95	-95.62	-95.46
Density kmol/cum	969.50	783.85	825.56	824.29

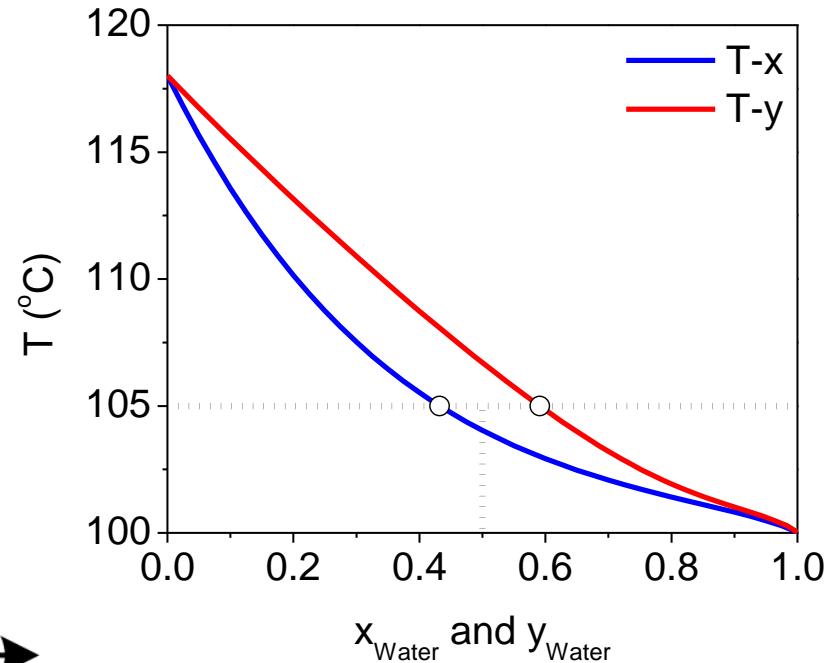
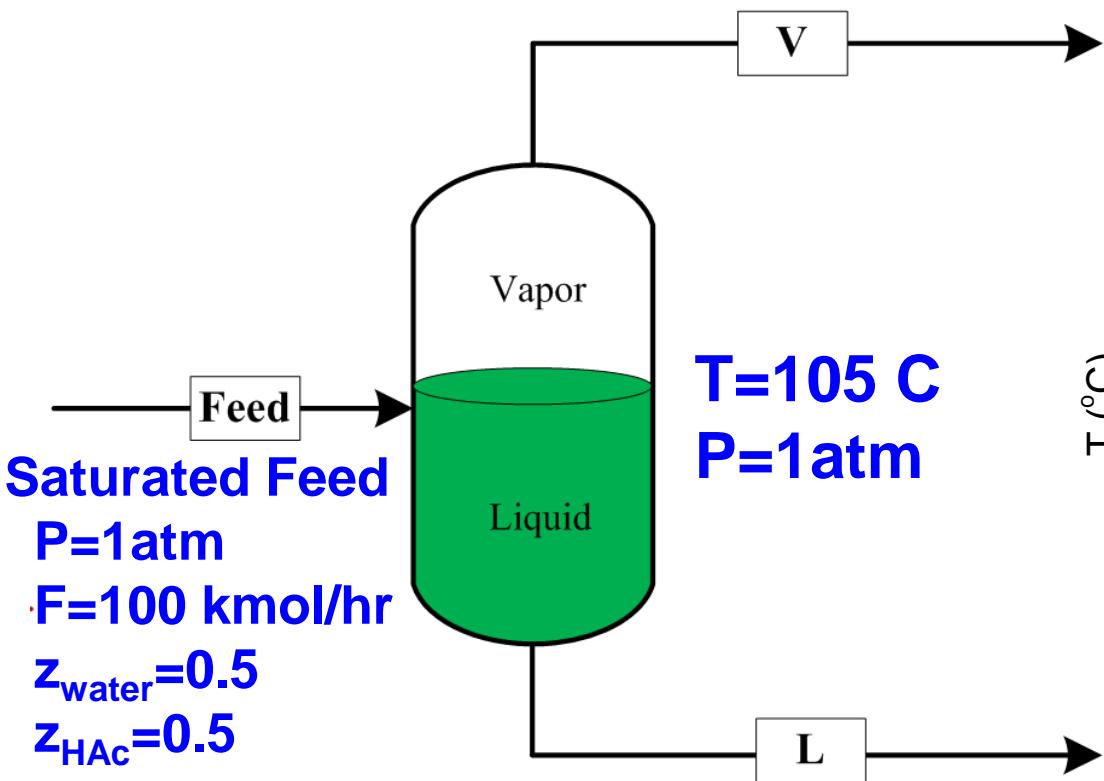
Exercise



	1	2	3	4	5	6
Mole Flow kmol/hr						
Water	10	0	0	?	?	?
Ethanol	0	5	0	?	?	?
Methanol	0	0	15	?	?	?
Total Flow kmol/hr	10	15	15	?	?	?
Temperature C	50	70	40	?	?	?
Pressure bar	1	1	1	1	4	2
Enthalpy kcal/mol	?	?	?	?	?	?
Entropy cal/mol-K	?	?	?	?	?	?
Density kmol/cum	?	?	?	?	?	?

Please use Peng-Robinson EOS to solve this problem.

Example 2: Flash Separation



What are flowrates and compositions of the two outlets?

Input Components

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Components Specifications - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Specifications Selection Petroleum Nonconventional Enterprise Database

Define components

Component ID	Type	Component name	Formula
HAC	Conventional	ACETIC-ACID	C2H4O2-1
WATER	Conventional	WATER	H2O
*			

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators

Material STREAMS Mixer FSPLIT SPLIT

For Help, press F1 C:\...AspenTech\Aspen Plus V7.1 Flowsheet Not Complete

Thermodynamic Model: NRTL-HOC

The screenshot shows the Aspen Plus V7.1 software interface. The title bar reads "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Specifications - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The main window is titled "Specifications" and displays a tree view of specification categories:

- Setup
- Components
- Properties
- Specifications** (selected)
- Property Methods
- Estimation
- Molecular Structure
- Parameters
- Data
- Analysis
- Prop-Sets
- Advanced
- CAPE-OPEN Packages
- Flowsheet
- Streams
- Blocks

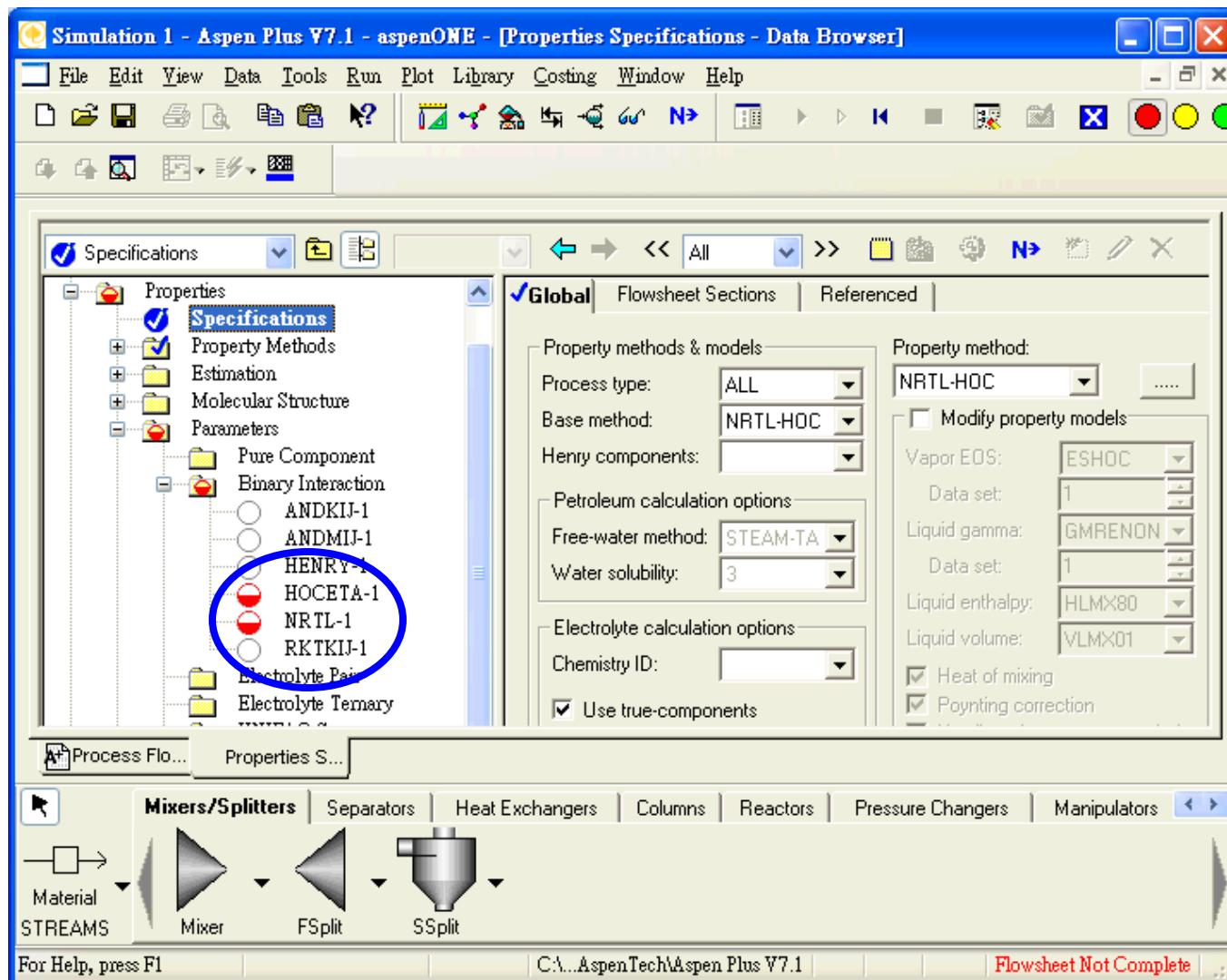
The "Global" tab is selected in the properties panel, showing the following settings:

- Property methods & models
 - Process type: ALL
 - Base method: NRTL-HOC
 - Henry components: (dropdown menu)
- Petroleum calculation options
 - Free-water method: STEAM-TA
 - Water solubility: 3
- Electrolyte calculation options
 - Chemistry ID: (dropdown menu)
- Property method: NRTL-HOC
 - Modify property models (checkbox)
 - Vapor EOS: ESHOC
 - Data set: 1
 - Liquid gamma: GMRENON
 - Data set: 1
 - Liquid enthalpy: HLMX80
 - Liquid volume: VLMX01
 - Heat of mixing (checkbox)
 - Poynting correction (checkbox)

At the bottom, there are tabs for "Process Flow..." and "Properties S...". Below the tabs, there is a toolbar with icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT, and tabs for Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, and Manipulators.

The status bar at the bottom left says "For Help, press F1". The bottom center says "C:\...AspenTech\Aspen Plus V7.1". The bottom right says "Flowsheet Not Complete".

Check Binary Parameters



Association parameters of HOC

The screenshot shows the Aspen Plus V7.1 software interface. The title bar reads "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Binary Interaction HOCETA-1 (SCAL...)]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The main window displays the "Properties Parameters Binary Interaction HOCETA-1 (SCAL...)" dialog. On the left, a tree view shows the following structure under "HOCETA-1":

- Properties
- Specifications
- Property Methods
- Estimation
- Molecular Structure
- Parameters
 - Pure Component
 - Binary Interaction
 - ANDKIJ-1
 - ANDMIJ-1
 - HENRY-1
 - HOCETA-1** (selected, highlighted with a blue oval)
 - NP-TL-1
 - RKTkJ-1
 - Electrolyte Pair
 - Electrolyte Ternary

The right panel shows the "Input" tab with the following settings:

- Parameter: HOCETA
- Data set: 1
- Units: (dropdown menu)

Under "Binary parameters", there is a table:

Component i	Component j	Component j	Component j
HAC	HAC	WATER	
HAC	4.500000000	2.500000000	
WATER	2.500000000	1.700000000	
*			

At the bottom, there are tabs for "Process Flow..." and "Properties P...". The tool palette at the bottom includes icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT.

Binary Parameters of NRTL

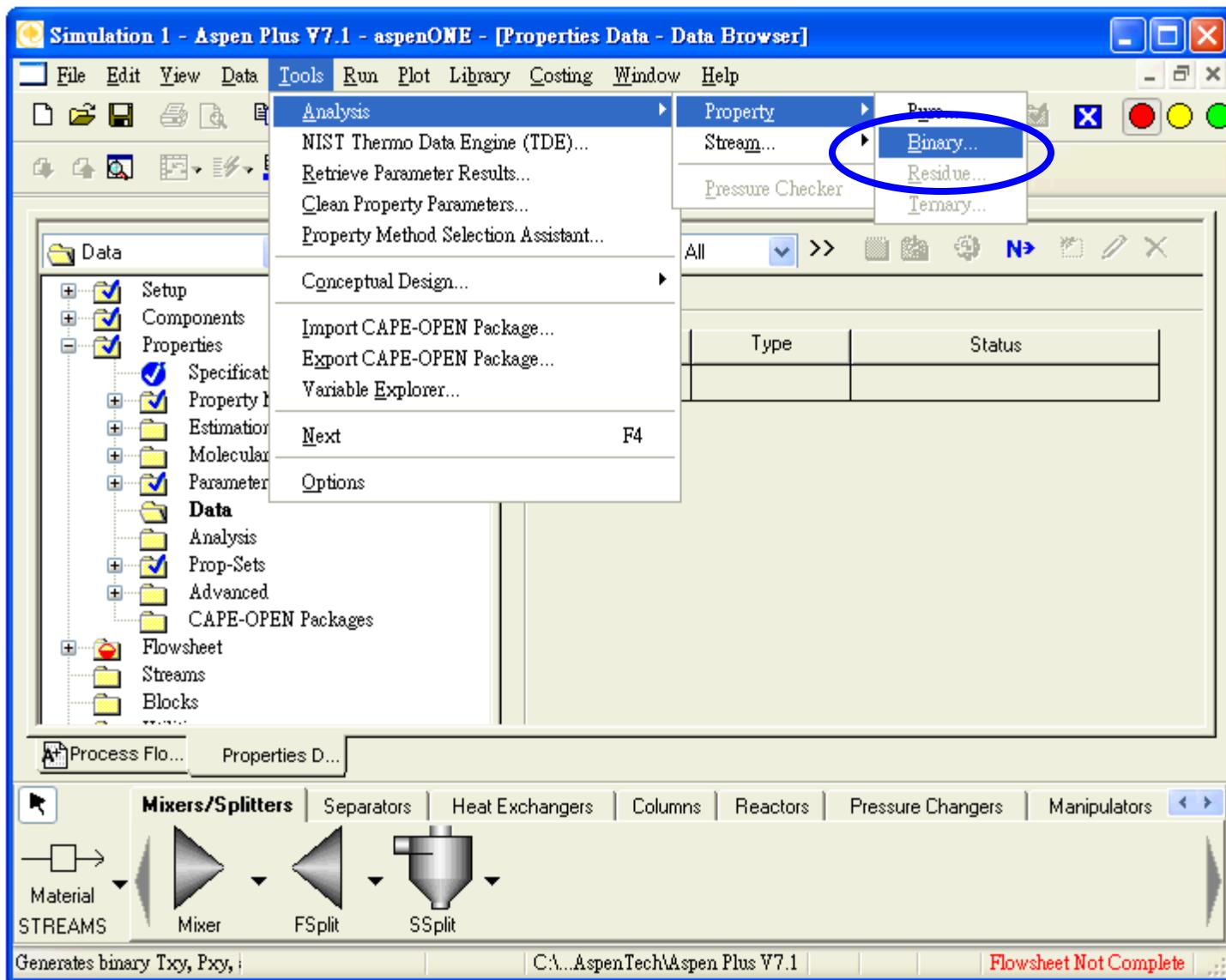
The screenshot shows the Aspen Plus V7.1 software interface. The title bar reads "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Parameters Binary Interaction NRTL-1 (T-DEPE...)]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The main window displays the "NRTL-1" properties dialog. On the left, a tree view shows checked nodes: Properties, Specifications, Property Methods, Estimation, Molecular Structure, Parameters, Pure Component, Binary Interaction (with sub-options ANDKIJ-1, ANDMIJ-1, HENRY-1, HOCTETA-1, NRTL-1, RKTKU-1), Electrolyte Pair, and Electrolyte Ternary. The "NRTL-1" node is highlighted with a blue oval. The right panel has tabs for Input and Databanks, with "Input" selected. It shows the "Parameter" set to "NRTL" and "Data set" set to "1". Below this, a table lists temperature-dependent binary parameters for components HAC and WATER at unit "C". The table includes columns for Component i, Component j, Temperature units, Source, AIJ, AJI, BIJ, and BJI. The "Source" dropdown is set to "APV71 VLE-I".

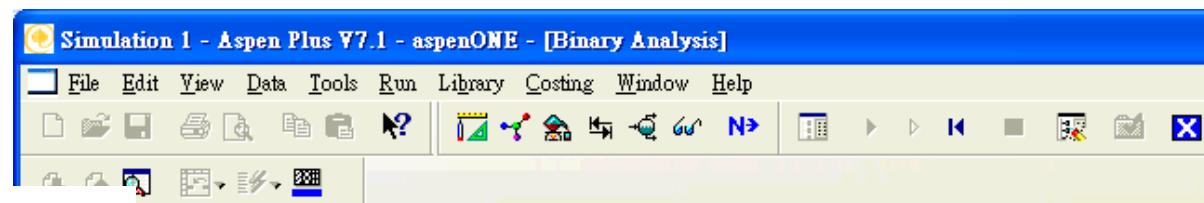
At the bottom, there are tabs for Process Flow, Properties P..., Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, and Manipulators. The Mixers/Splitters tab is active, showing icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT.

The status bar at the bottom indicates "C:\...\AspenTech\Aspen Plus V7.1" and "Flowsheet Not Complete".

Binary Analysis



T-xy plot



1. Select analysis type (Txy)

2. Select phase (VLE, VLLE)

2. Select two component

5. Specify pressure

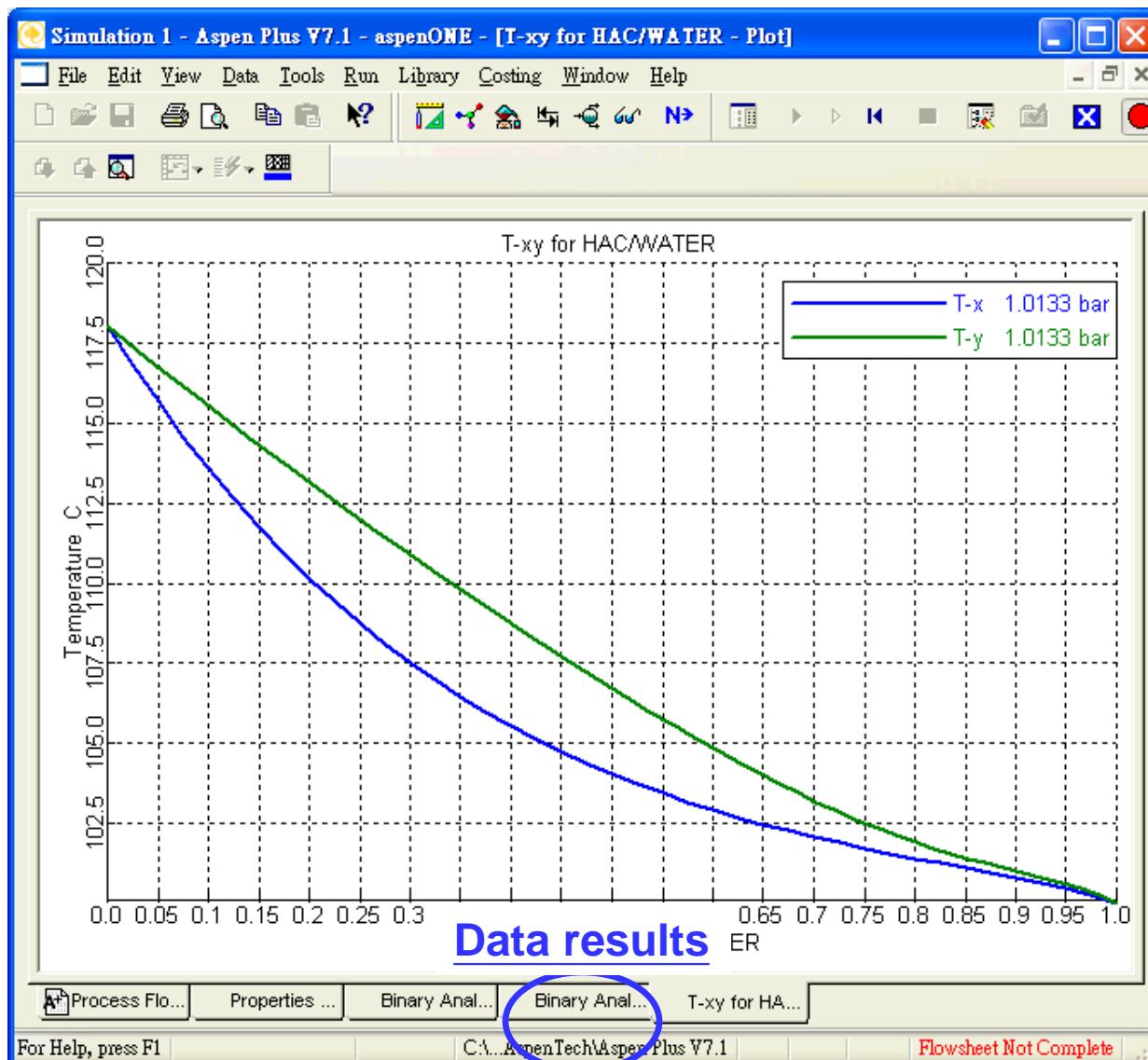
3. Select compositions basis

6. Select property method

4. Specify composition range

7. click Go to generate the results

Calculation Result of T-xy



Generate xy plot

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Binary Analysis Results]

File Edit View Data Tools Run Plot Library Costing Window Help

Binary analysis results

PRES	MOLEFRAC WATER	TOTAL TEMP	TOTAL KVL HAC	TOTAL KVL WATER
bar		C		
1.01325	0	118.0085	1.000003	1.963938
1.01325	0.025	116.7958	0.9761976	1.928255
1.01325	0.05	115.6551	0.9530605	1.891854
1.01325	0.075	114.583	0.930679	1.854972
1.01325	0.1	113.5764	0.9091306	1.817833
1.01325	0.125	112.6322	0.8884803	1.780637
1.01325	0.15	111.7473	0.8687866	1.743571
1.01325	0.175	110.9187	0.8500892	1.706789

Plot Wizard

Plot Wizard Step 2

To begin, select a plot type you wish to generate.

Click on a plot type

TXY TX YX Gamma

KVL

Click on the Next button to continue.

Click on the Finish button to generate a plot with default settings.

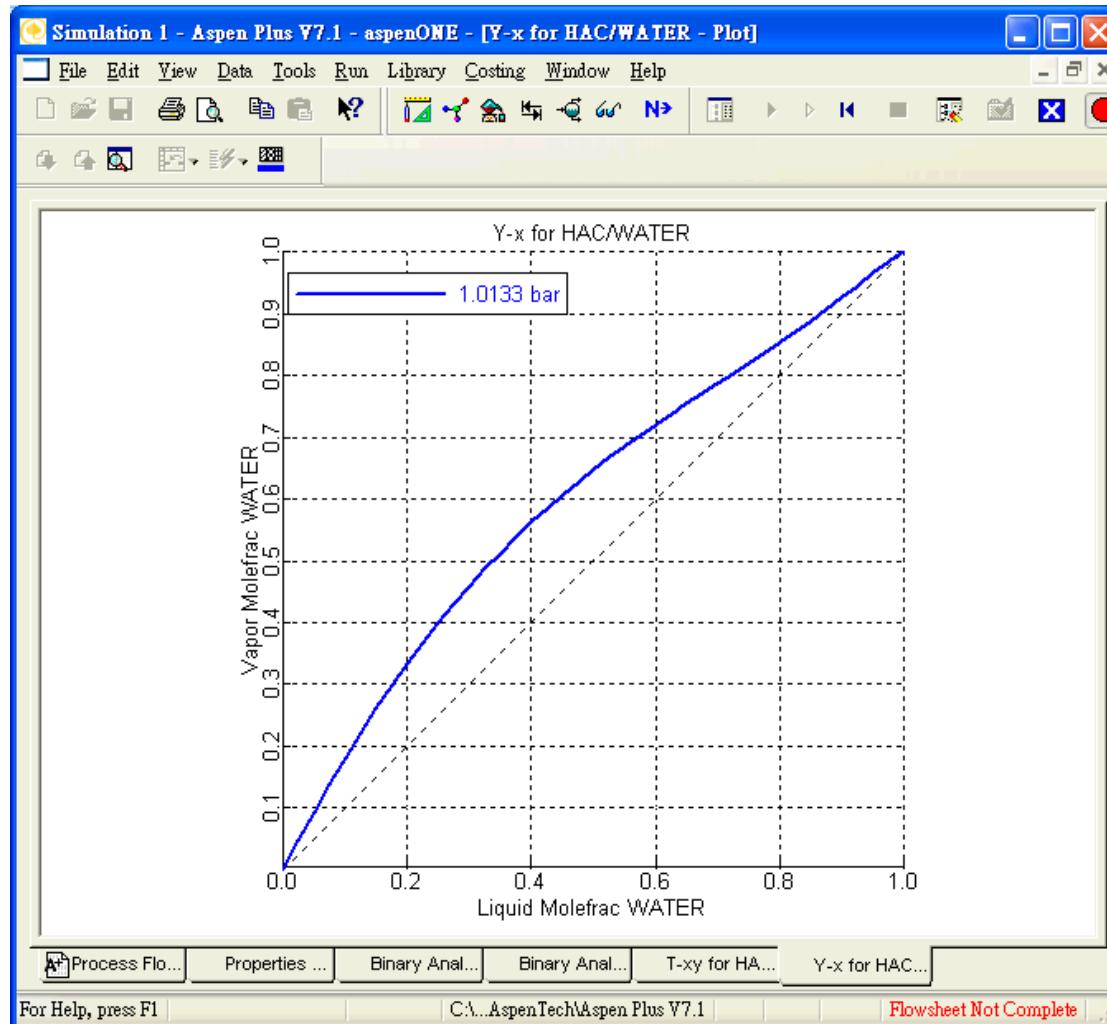
Help Cancel <Back Next> Finish

Process Flo... Properties ... Binary Anal... **Binary Analy...** T-xy for HA...

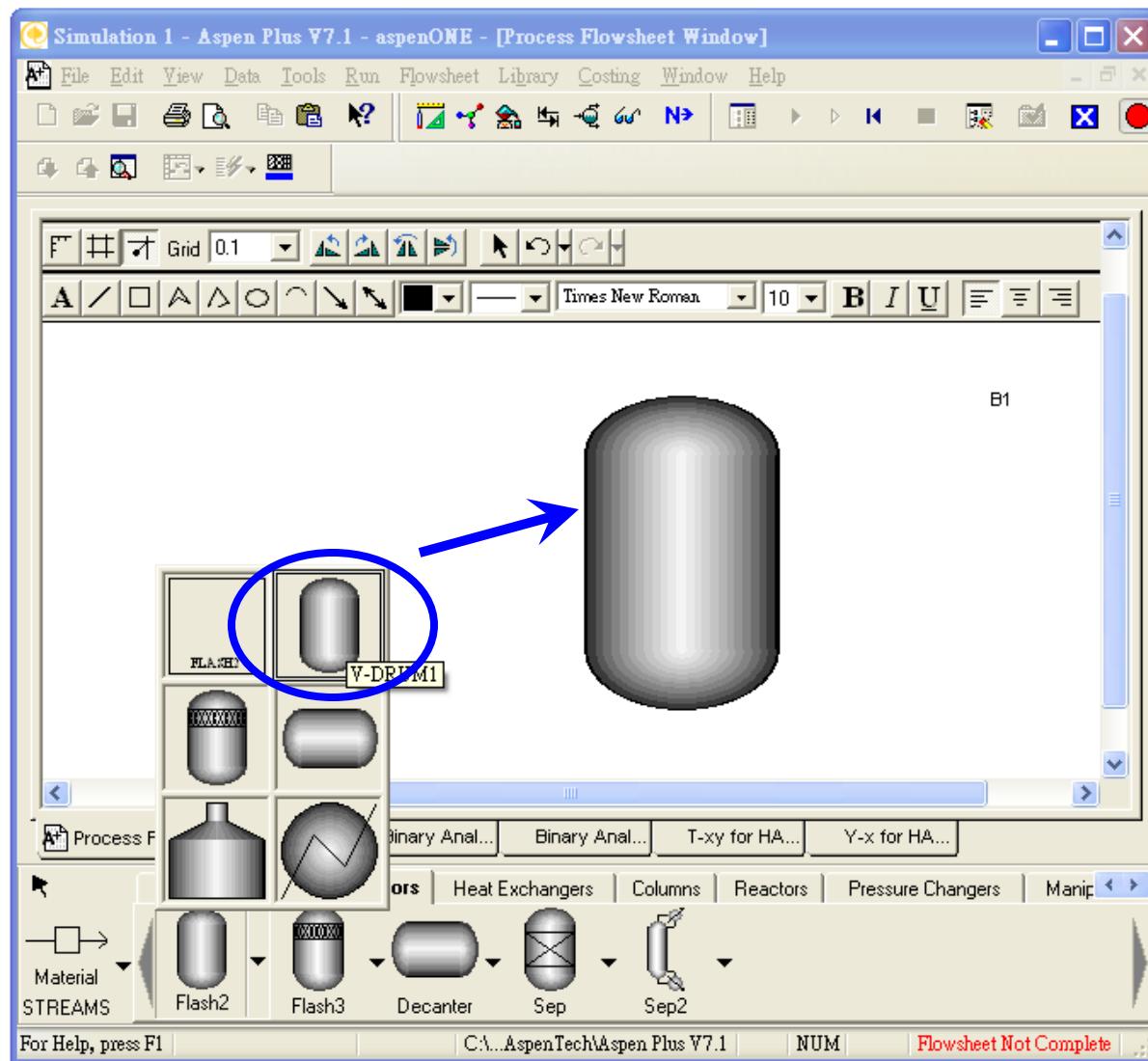
For Help, press F1 C:\AspenTech\Aspen Plus V7.1 Flowsheet Not Complete

aspen tech process, to the power of e.

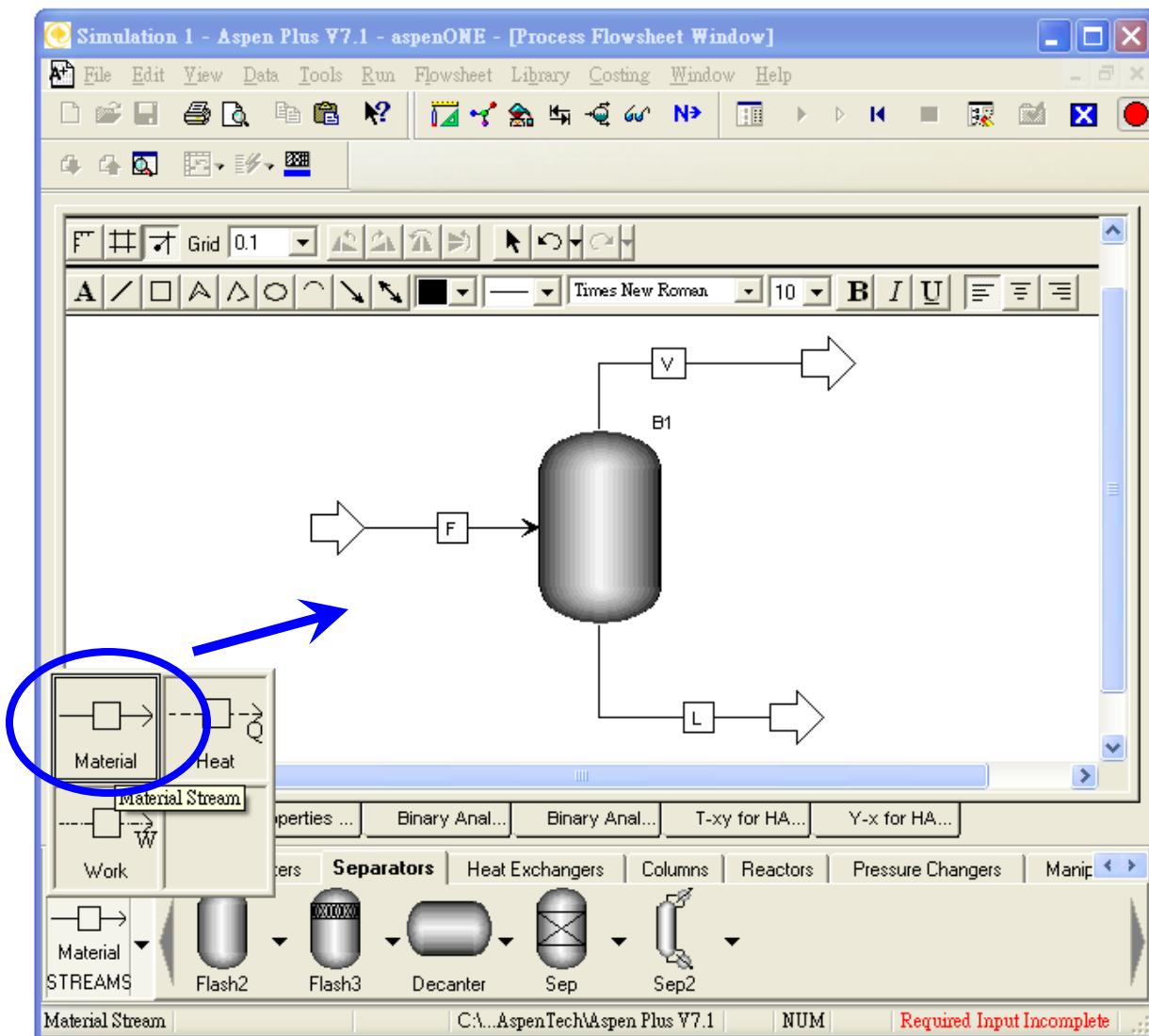
Generate xy plot (cont'd)



Add Block: Flash2



Add Material Stream



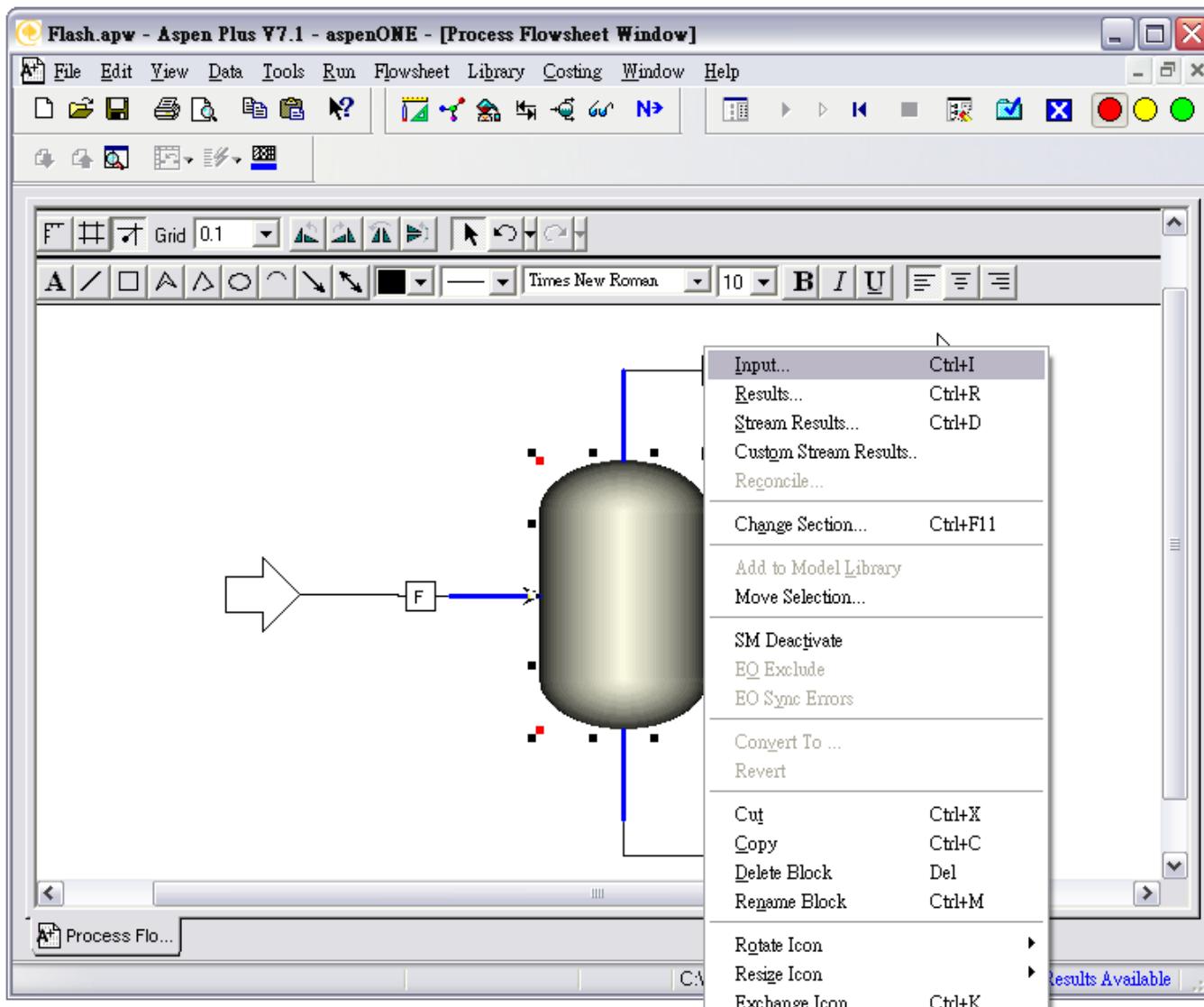
Specify Feed Condition

The screenshot shows the Aspen Plus V7.1 Data Browser interface. The left pane displays a tree view of simulation objects, with 'Streams' expanded to show 'F' (selected), 'Input', 'Results', 'EO Variables', and 'Custom Stream Results'. The right pane is titled 'Specifications' and contains fields for 'Substream name' (set to 'MIXED'), 'State variables' (Vapor fraction: 0, Pressure: 1 atm), 'Composition' (Mole-Frac: HAC=0.5, WATER=0.5), and 'Total flow' (100 kmol/hr). A blue box highlights the 'Vapor fraction=0' entry. Below the browser are toolbars for Process Flow, Properties, Binary Analysis, and T-xy for HAc.

**Saturated Feed
(Vapor fraction=0)**

P=1atm
F=100 kmol/hr
 $z_{\text{water}}=0.5$
 $z_{\text{HAc}}=0.5$

Block Input: Flash2



Flash2: Specification

The screenshot shows the Aspen Plus V7.1 Data Browser interface. The title bar reads "Simulation 1 - Aspen Plus V7.1 - aspenONE - [Block B1 (Flash2) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The left pane displays a tree view of the simulation structure:

- Setup
- Components
- Properties
- Flowsheet
- Streams
- Blocks
 - B1
 - Input
 - Hcurves
 - Dynamic
 - Block Options
 - Results
 - EO Variables
 - EO Input
 - Spec Groups
 - Ports
 - Stream Results
 - Custom Stream Results
 - Utilities
 - Reactions
 - Convergence
 - Flowsheeting Options
 - Model Analysis Tools
 - EO Configuration
 - Results Summary

The right pane is titled "Specifications" and contains the following settings:

 - Flash specifications:
 - Temperature: 105 C
 - Pressure: 1 atm
 - Valid phases: Vapor-Liquid

A large blue callout box highlights the temperature and pressure settings with the text "T=105 C" and "P=1atm". A note at the bottom of the pane states: "Let you type the pressure. Absolute units: outlet pressure if value > 0; pressure drop if value <= 0. pressure for all values. See Help."

The bottom navigation bar includes tabs for Process Fl..., Properties..., Binary An..., T-xy for H..., Y-x for H..., Streams - ..., Block B1 (F...), and a status message "Required Input Incomplete".

Required Input Complete

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Properties Analysis - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Analysis

- Setup
- Components
- Properties
 - Specifications
 - Property Methods
 - Estimation
 - Molecular Structure
 - Parameters
 - Data
 - Analysis**
 - Prop-Sets
 - Advanced
 - CAPE-OPEN Packages
- Flowsheet
- Streams
- Blocks
- Utilities
- Reactions
- Connections

Object manager

Name	Type	Status

New... Edit Delete Copy

Process Flo... Properties... Properties... Properties A...

For Help, pre C:\AspenTech\Aspen Plus V7.1 NUM Required Input Complete

Click ► to run simulation

****Before running simulation, property analysis should be closed.**

Stream Results

Simulation 1 - Aspen Plus V7.1 - aspenONE - [Process Flowsheet Window]

File Edit View Data Tools Run Flowsheet Library Costing Window Help

Stream Results... Ctrl+D

Temperature C 104.0 105.0 105.0

Pressure bar 1.013 1.013 1.013

Vapor Frac 0.000 1.000 0.000

Mole Flow kmol/hr 100.000 42.658 57.342

Mass Flow kg/hr 3903.392 1501.859 2401.533

Volume Flow cum/hr 4.301 1129.862 2.631

Enthalpy MMkcal/hr -8.991 -3.304 -5.333

Mole Flow kmol/hr

HAC 50.000 17.445 32.555

WATER 50.000 25.213 24.787

Mole Frac

HAC 0.500 0.409 0.568

WATER 0.500 0.591 0.432

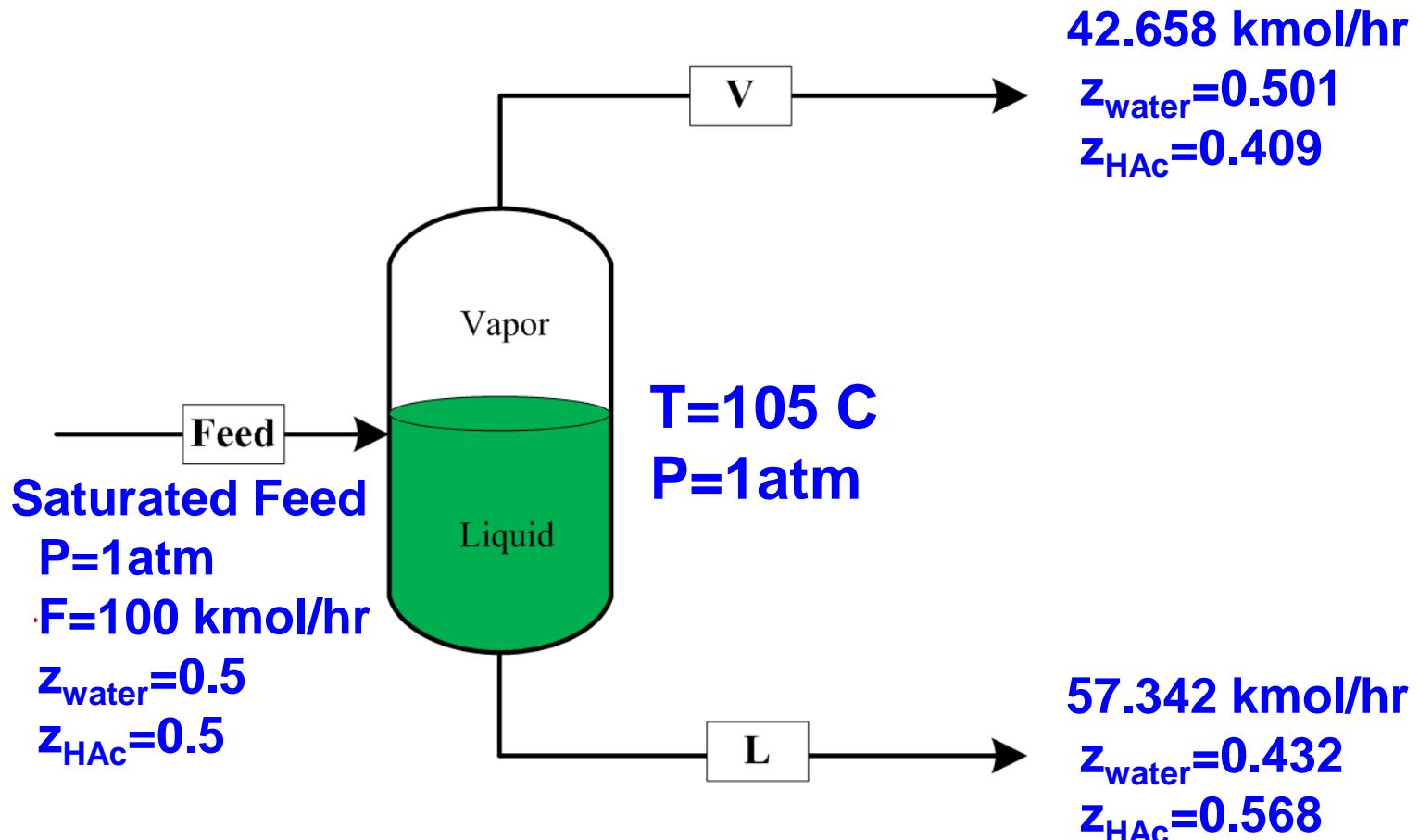
Cut Available

Process Flo... Control Panel Properties ... Properties ...

aspenTech

The screenshot shows the Aspen Plus V7.1 software interface. A process flowsheet window is open, featuring a central vessel component with two streams entering from the left and exiting to the right. A context menu is displayed over the vessel, with the 'Stream Results...' option highlighted. To the right of the flowsheet is a 'Stream Table' dialog box. The table has columns for Stream ID (F, V, L), Temperature (C), Pressure (bar), and other properties like Vapor Frac, Mole Flow (kmol/hr), Mass Flow (kg/hr), Volume Flow (cum/hr), Enthalpy (MMkcal/hr), and Mole Frac. The table lists data for stream 'GEN_M' across four rows.

Stream Results (cont'd)



HEAT EXCHANGE

熱物流

入口溫度：200°C、入口壓力：0.4 MPa

流量：10000kg/hr

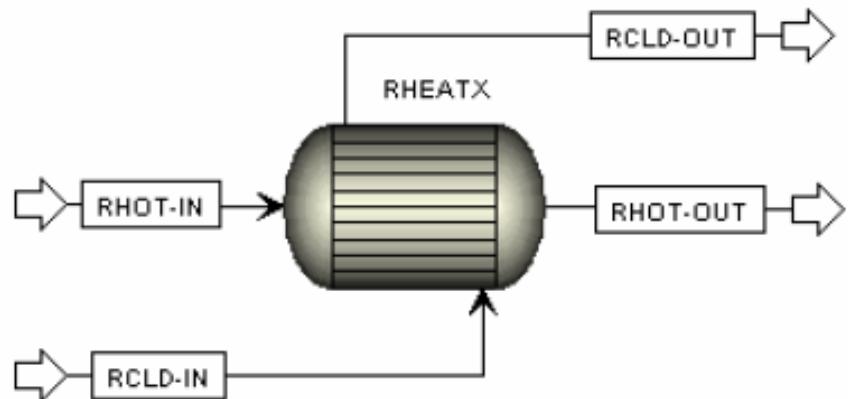
組成：苯 50%，苯乙烯 20%，水 10%

冷卻水

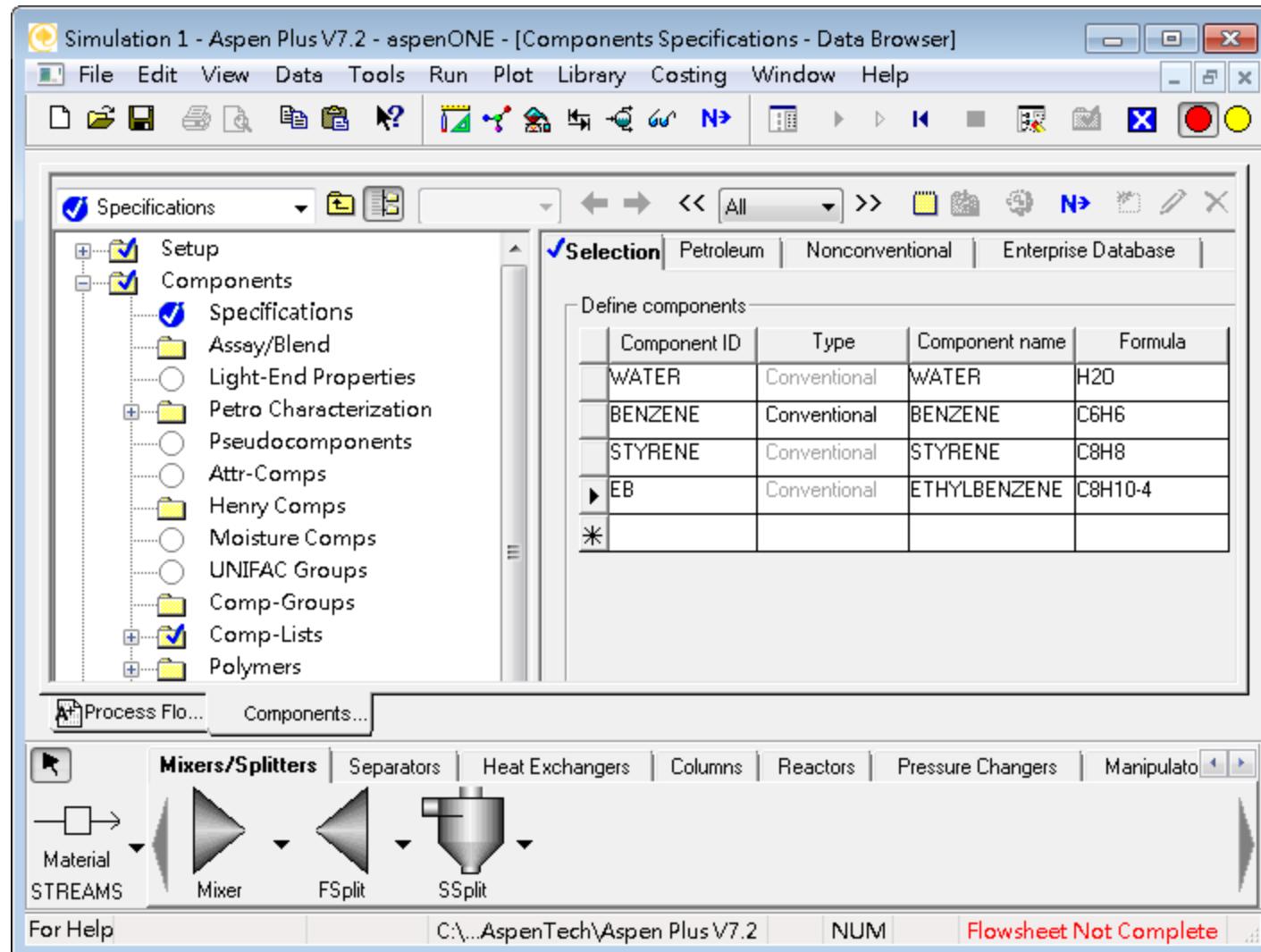
入口溫度：20°C、入口壓力：1.0 MPa

流量：60000 kg/hr。

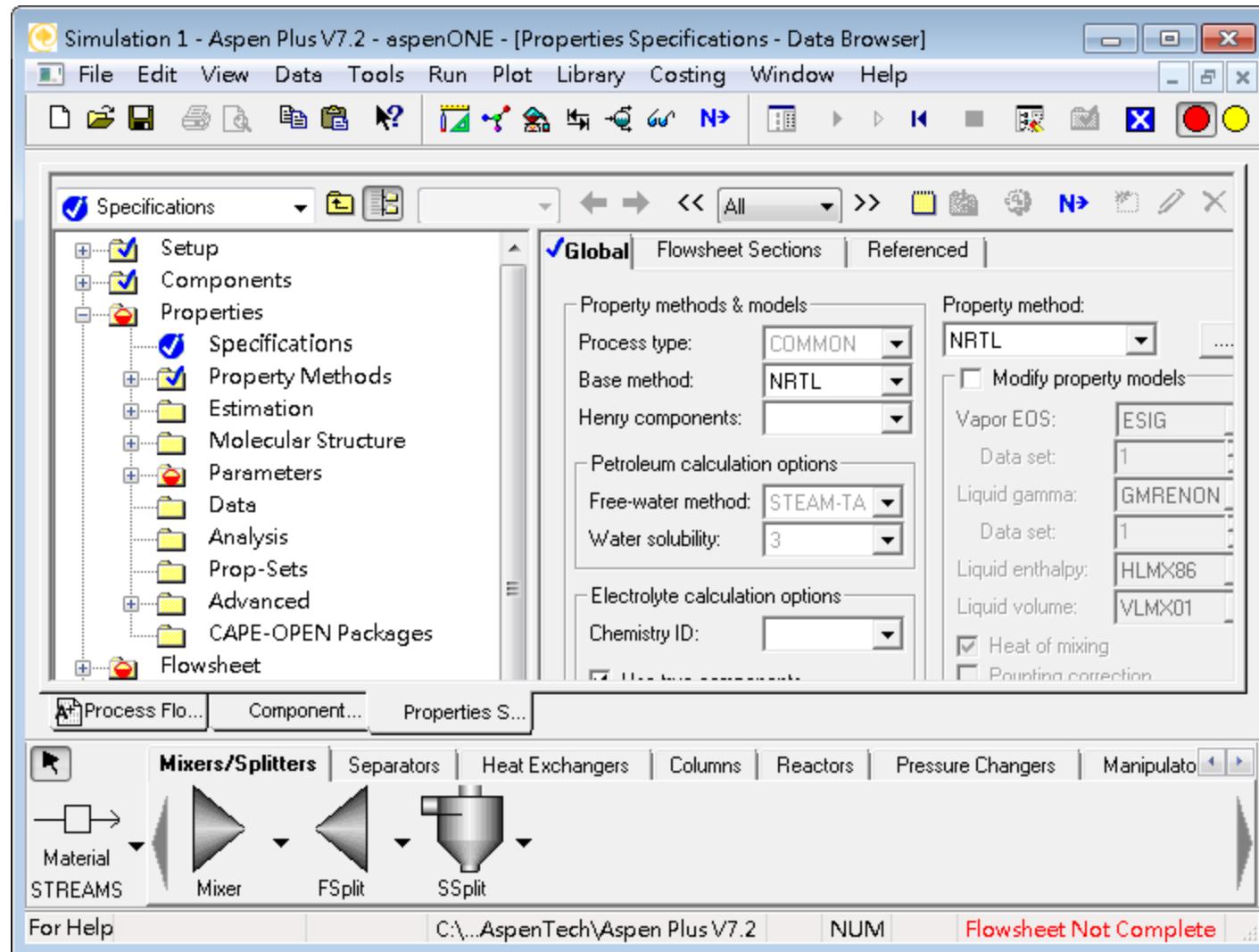
熱流出口氣相分率為 0
(飽和液相)



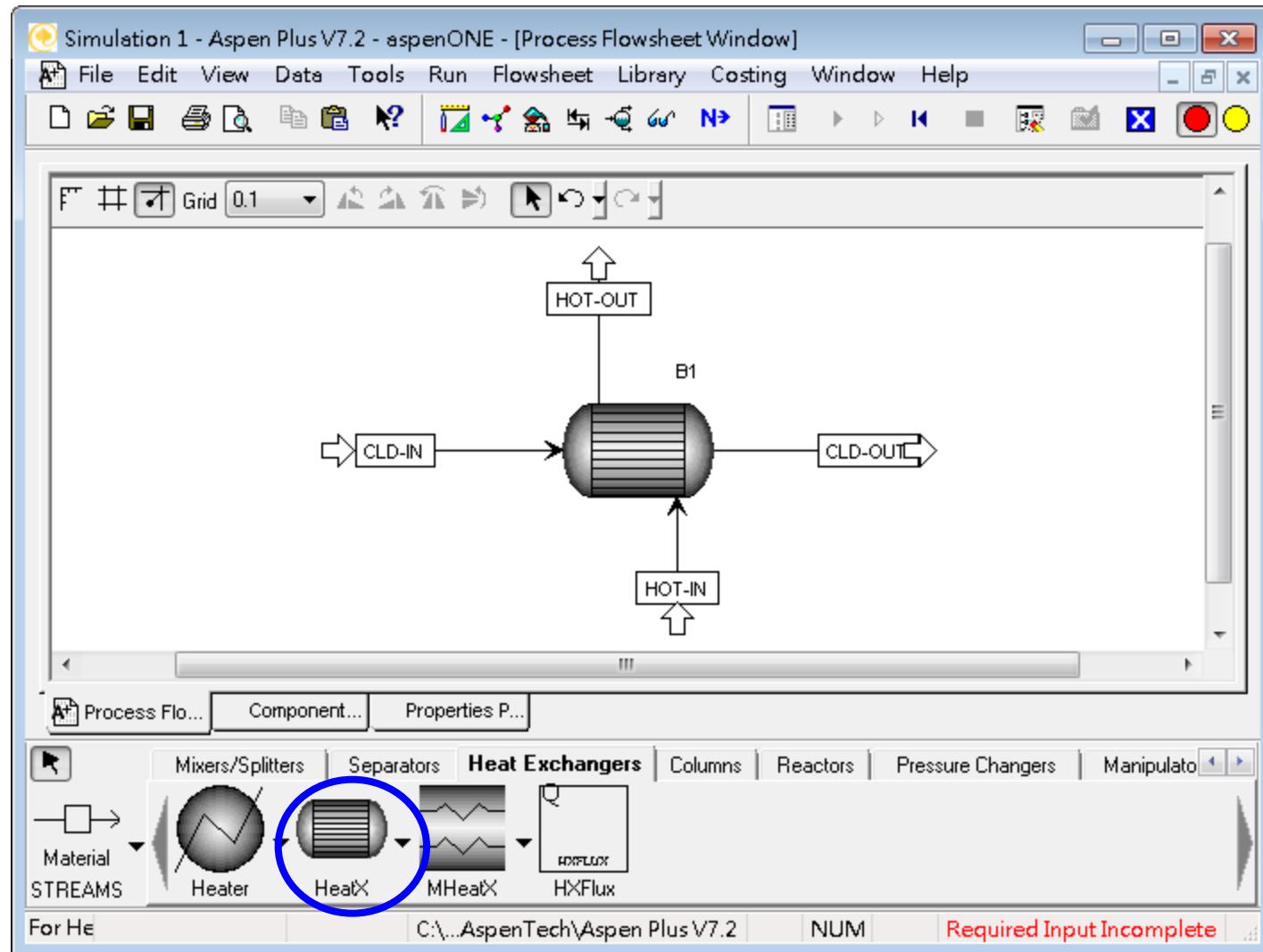
COMPONENTS – SPECIFICATION



Thermodynamic Model – NRTL



ADD BLOCK: HEATX



Feeds Conditions

CLD-IN

✓Specifications | Flash Options | PSD | Component Attr. | EO Optio

Substream name: ✓MIXED Ref Temperature

State variables

Temperature	20	C
Pressure	10	bar
Total flow:	Mass	60000 kg/hr

Composition

Component	Value
WATER	1
BENZENE	
STYRENE	
EB	

HOT-IN

✓Specifications | Flash Options | PSD | Component Attr. | EO Optio

Substream name: ✓MIXED Ref Temperature

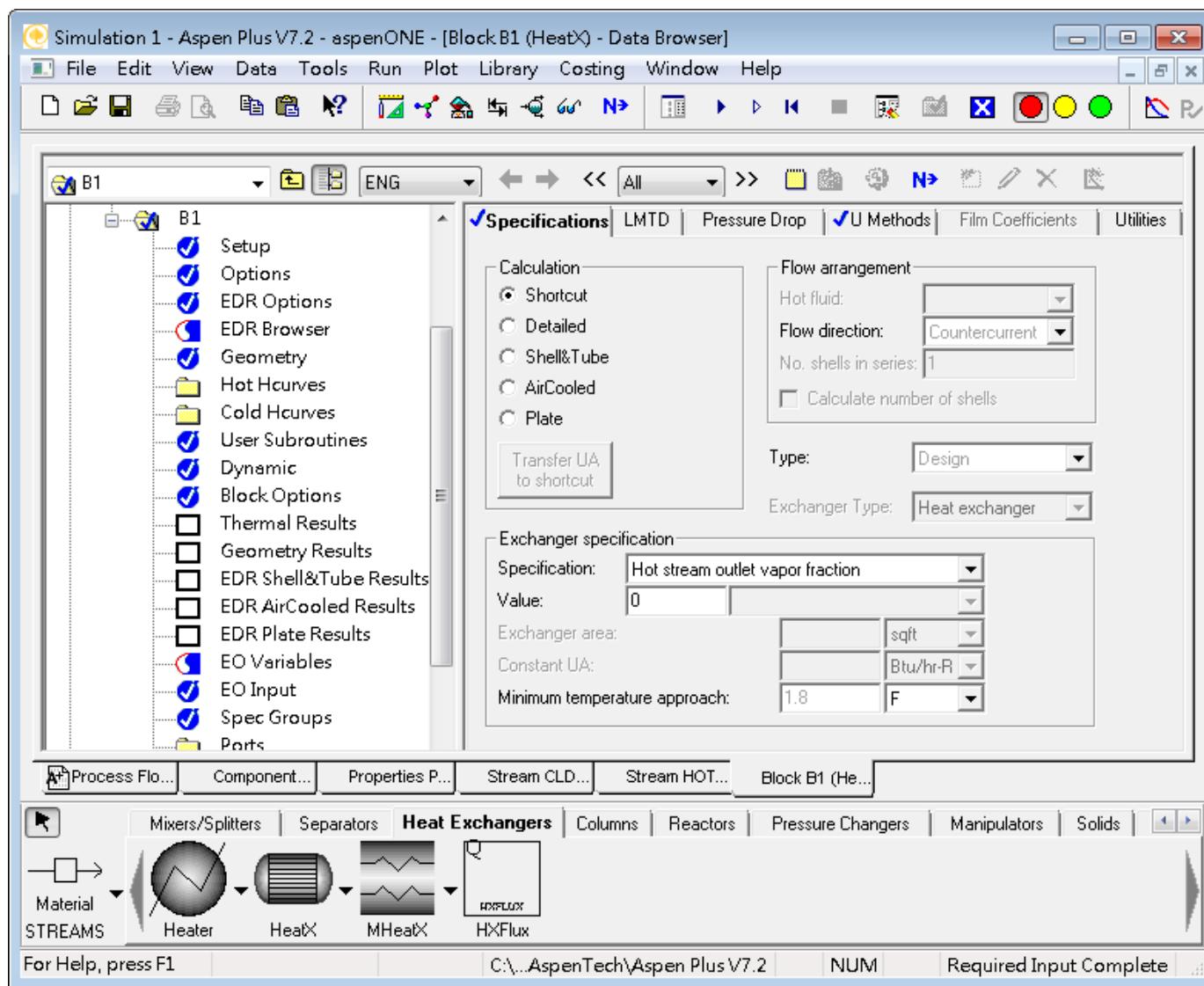
State variables

Temperature	200	C
Pressure	4	bar
Total flow:	Mass	10000 kg/hr

Composition

Component	Value
WATER	0.1
BENZENE	0.5
STYRENE	0.2
EB	0.2

BLOCK INPUT



Check result

		Display: All streams	Format: FULL	Stream Table	
		CLD-IN	CLD-OUT	HOT-IN	HOT-OUT
Substream: MIXED					
Mole Flow kmol/hr					
WATER	3330.506	3330.506	55.50843	55.50843	
BENZENE	0.0	0.0	64.00931	64.00931	
STYRENE	0.0	0.0	19.20279	19.20279	
EB	0.0	0.0	18.83817	18.83817	
Mass Flow kg/hr					
WATER	60000.00	60000.00	1000.000	1000.000	
BENZENE	0.0	0.0	5000.000	5000.000	
STYRENE	0.0	0.0	2000.000	2000.000	
EB	0.0	0.0	2000.000	2000.000	
Mass Frac					
WATER	1.000000	1.000000	.1000000	.1000000	
BENZENE	0.0	0.0	.5000000	.5000000	
STYRENE	0.0	0.0	.2000000	.2000000	
EB	0.0	0.0	.2000000	.2000000	
Total Flow kmol/hr	3330.506	3330.506	157.5587	157.5587	
Total Flow kg/hr	60000.00	60000.00	10000.00	10000.00	
Total Flow l/min	1001.234	1029.187	25826.01	200.9999	
Temperature K	293.1500	320.9937	473.1500	376.3495	
Pressure atm	9.869233	9.869233	3.947693	3.947693	
Vapor Frac	0.0	0.0	1.000000	0.0	
Liquid Frac	1.000000	1.000000	0.0	1.000000	
Solid Frac	0.0	0.0	0.0	0.0	
Enthalpy cal/mol	-68314.18	-67847.77	-3206.225	-13065.37	
Enthalpy cal/gm	-3792.013	-3766.123	-50.51687	-205.8562	

Check result

Simulation 1 - Aspen Plus V7.2 - aspenONE - [Block B1 (HeatX) Thermal Results - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Streams Blocks B1 EDR Browser Thermal Results Geometry Results EDR Shell&Tube Results EDR AirCooled Results EDR Plate Results EO Variables Stream Results Custom Stream Results EO Configuration Results Summary

Summary Balance Exchanger Details Pres Drop/Velocities Zones Utility Us

Heatx results

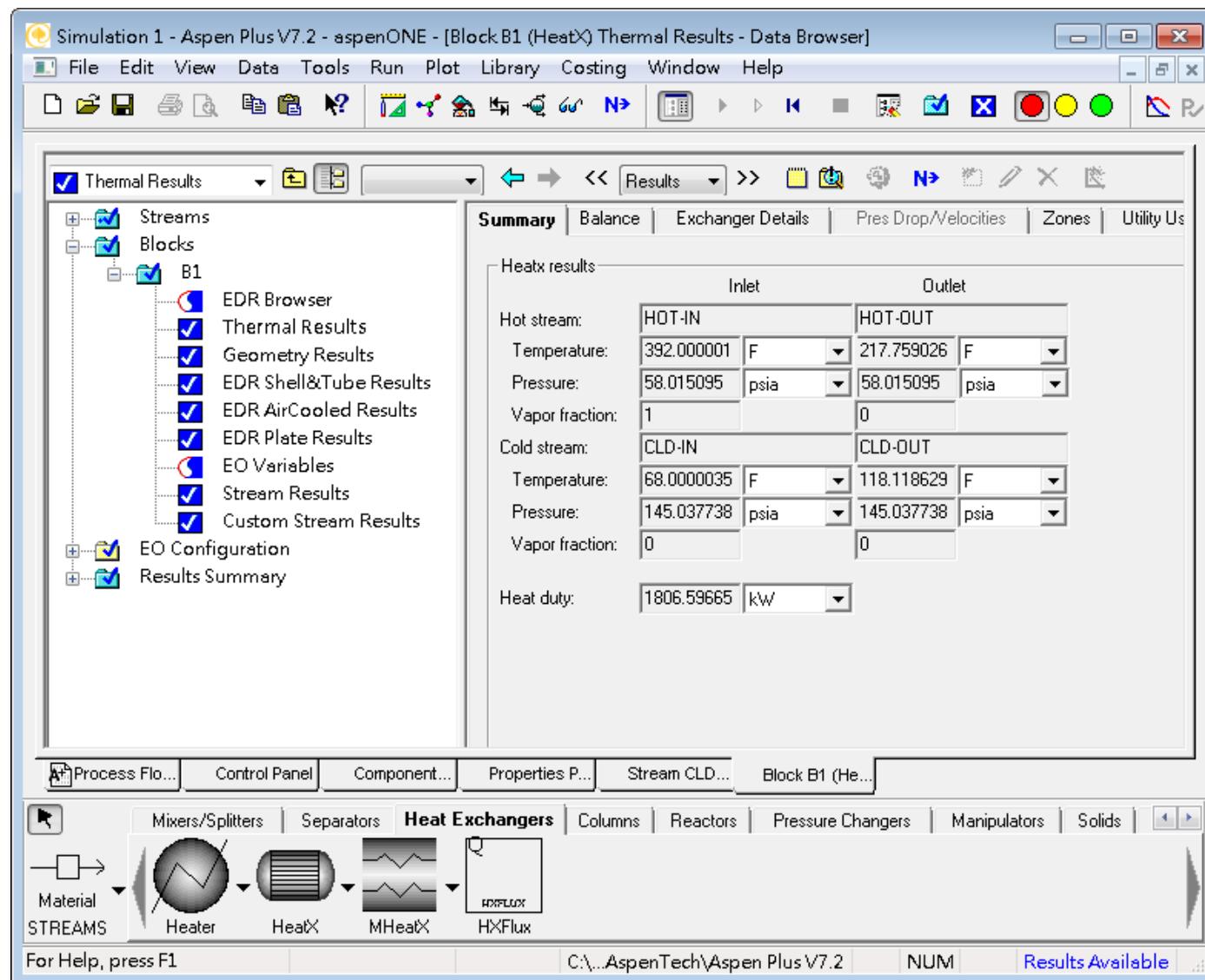
	Inlet	Outlet
Hot stream:	HOT-IN	HOT-OUT
Temperature:	392.000001 F	217.759026 F
Pressure:	58.015095 psia	58.015095 psia
Vapor fraction:	1	0
Cold stream:	CLD-IN	CLD-OUT
Temperature:	68.0000035 F	118.118629 F
Pressure:	145.037738 psia	145.037738 psia
Vapor fraction:	0	0
Heat duty:	1806.59665 kW	

Process Flo... Control Panel Component... Properties P... Stream CLD... Block B1 (He...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids

Material STREAMS Heater HeatX MHeatX HXFlux

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Results Available



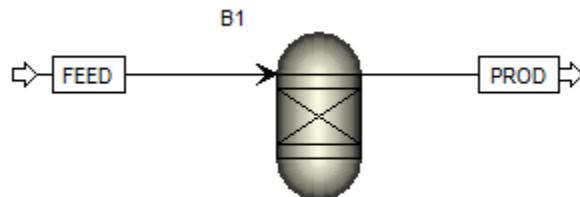
Introduction to Aspen Plus

Part 5: Running simulation

Reactor Systems

(RGIBBS, RPLUG,RCSTR)

Equilibrium Reactor: RGIBBS

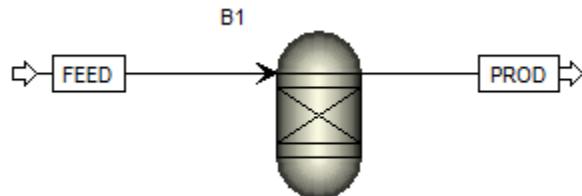


RGIBBS unit predicts the product by minimizing GIBBS energy in the system

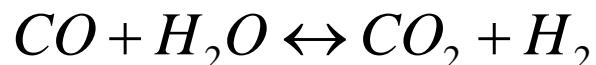
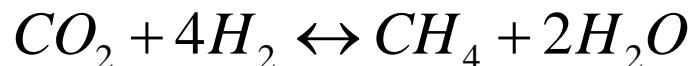
It is very Useful When...:

- 1. Reaction Kinetics are unknown.**
- 2. There are lots of products**

Equilibrium Reactor: RGIBBS



Reactions:

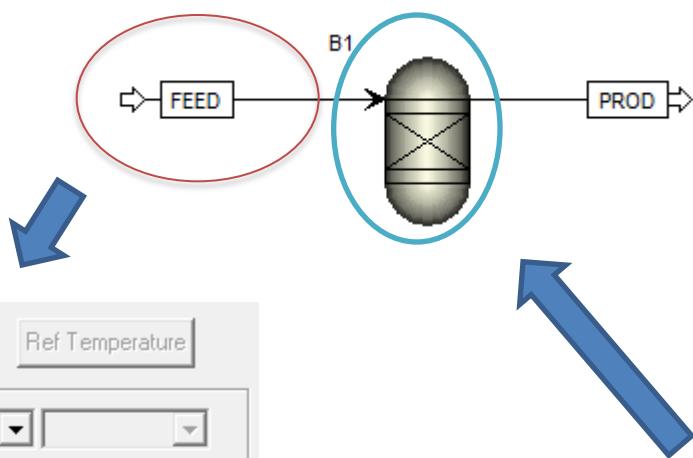


Fresh Feed	
Flow rate	1000 (kmol/h)
CO	0.2368
H ₂	0.7172
H ₂ O	0.0001
CH ₄	0.0098
CO ₂	0.0361

T=300 k

P=470 psia

Equilibrium Reactor: RGIBBS



Substream name: MIXED

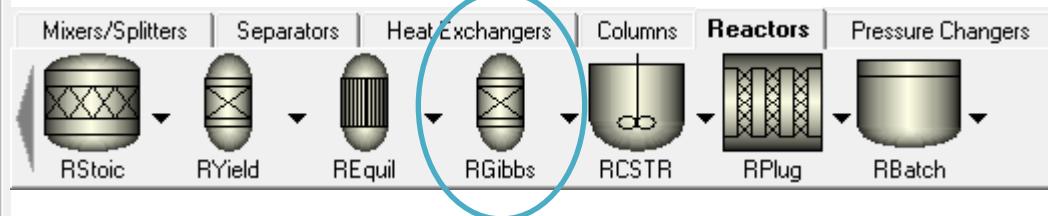
State variables

Temperature	300	K	
Pressure	470	psia	
Total flow:	Mole	1000	kmol/hr

Solvent:

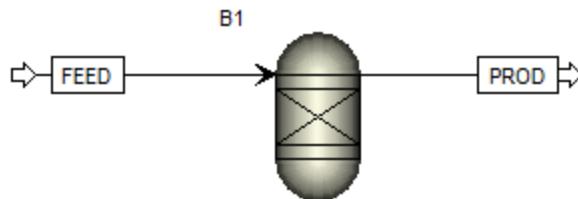
Composition

Mole-Frac	
Component	Value
CO	0.2368
H ₂ O	0.0001
CO ₂	0.0361
H ₂	0.7172
CH ₄	0.0098



Equilibrium Reactor: RGIBBS

Inside the Block:



✓ Specifications | Products | Assign Streams | Inerts | Restricted Equilibrium | Utility

Operating conditions

Pressure: 470 psia
Temperature: 300 K
Heat duty: Watt

Calculation options

Calculate phase equilibrium and chemical equilibrium
 Calculate phase equilibrium only
 Calculate phase equilibrium and chemical equilibrium
 Restrict chemical equilibrium - specify temperature approach or reactions
 Restrict chemical equilibrium - specify duty and temp. calc temp approach

Include vapor phase Solid Phases

Substreams

Merge all CISOLID species into the first CISOLID substream

✓ Specifications | Products | Assign Streams | Inerts | Restricted Equilibrium | Utility

RGibbs considers all components as products
 Identify possible products
 Define phases in which products appear

Hydrate-check: Rigorous

Products determined by RGibbs

RGibbs determines the phase of each product as fluid or solid based on its properties.

Check result

Material			
Display: Streams Format: GEN_E Stream Table			
	FEED	PROD	
Temperature K	300.0	300.0	
Pressure atm	31.98	31.98	
Vapor Frac	1.000	1.000	
Mole Flow kmol/hr	1000.000	523.000	
Mass Flow kg/hr	9826.426	9826.426	
Volume Flow l/min	12981.346	4727.868	
Enthalpy MMBtu/hr	-38.969	-86.434	
Mole Flow kmol/hr			
CO	236.800	TRACE	
H2O	0.100	240.300	
CO2	36.100	34.400	
H2	717.200	0.001	
CH4	9.800	248.300	
Mole Frac			
CO	0.237	TRACE	
H2O	100 PPM	0.459	
CO2	0.036	0.066	
H2	0.717	1 PPM	
CH4	0.010	0.475	

KINETICS REACTORS: RPLUG

Reaction :Exothermic & reversible



$$Rate = k_f Y_{CO} Y_{H_2O} - k_r Y_{CO_2} Y_{H_2} \left(\frac{kmol}{kgcat \times s} \right)$$

$$k_f = 51.545 \exp\left(\frac{-47400}{RT}\right)$$

$$k_r = 3922.1 \exp\left(\frac{-85458}{RT}\right)$$

Rate [=] Kmol/Kgcat/s

Activation Energy [=] KJ/Kmol

KINETICS REACTORS: RPLUG

Reaction :Exothermic & reversible



Fresh Feed	
Flow rate	200 (mol/h)
CO	0.030
H ₂	0.430
H ₂ O	0.392
CO ₂	0.148

Catalyst Loading = 0.1865 Kg

Bed Voidage = 0.8928

Feed Temperature = 583K

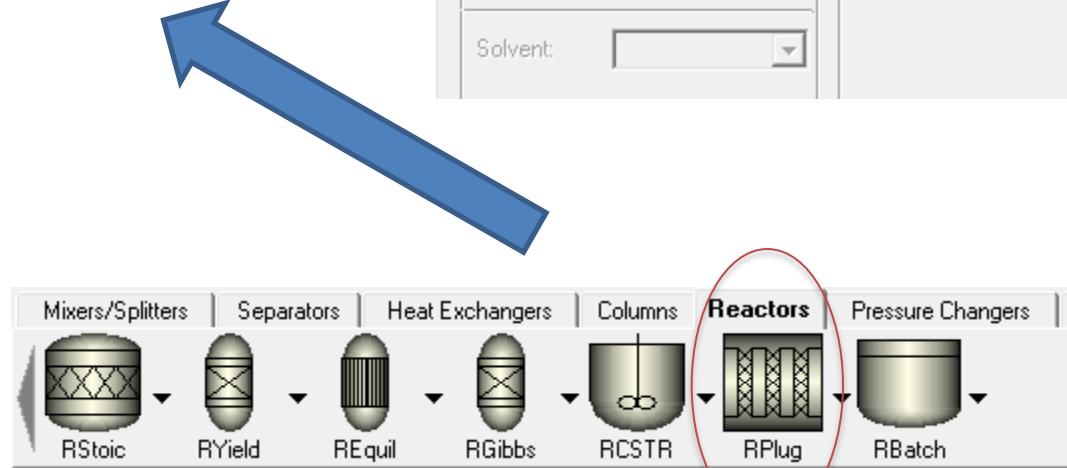
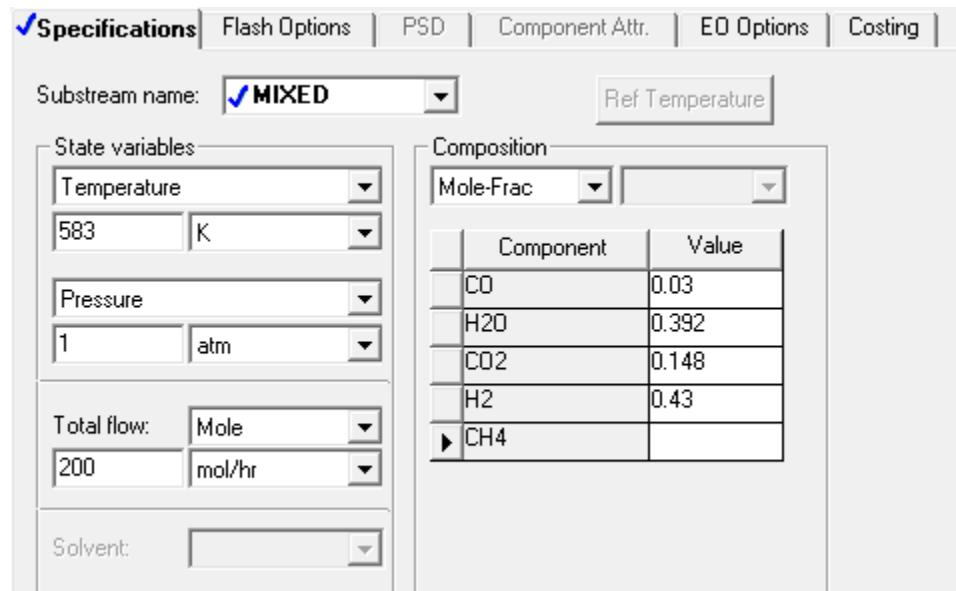
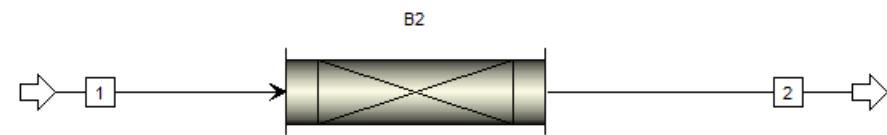
Feed Pressure = 1 bar

Reactor Length = 10 m

Reactor Diameter = 5m

KINETICS REACTORS: RPLUG

Feed Stream:



KINETICS REACTORS: RPLUG

Reaction Setting:

✓ Stoichiometry ✓ Kinetic Equilibrium Activity

1) CO + H₂O → CO₂ + H₂

Reacting phase: Vapor Rate basis: Cat (wt)

Power Law kinetic expression
Kinetic factor = $k(T/T_0)^n e^{-(E/R)[1/T - 1/T_0]}$

k:	51.545	
n:	0	
E:	47400	kJ/kmol
T ₀ :		K
[C _i] basis:	Mole fraction	

Edit reactions Solids

KINETICS REACTORS: RPLUG

Reaction Setting:

✓ Stoichiometry ✓ Kinetic Equilibrium Activity

2) $\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$

Reacting phase: Vapor Rate basis: Cat (wt)

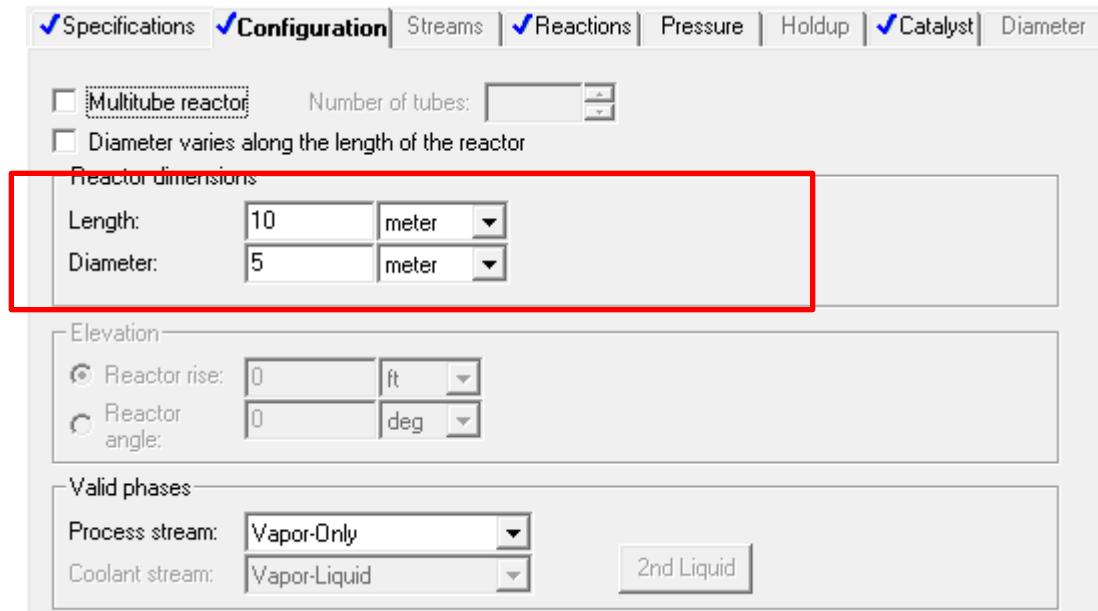
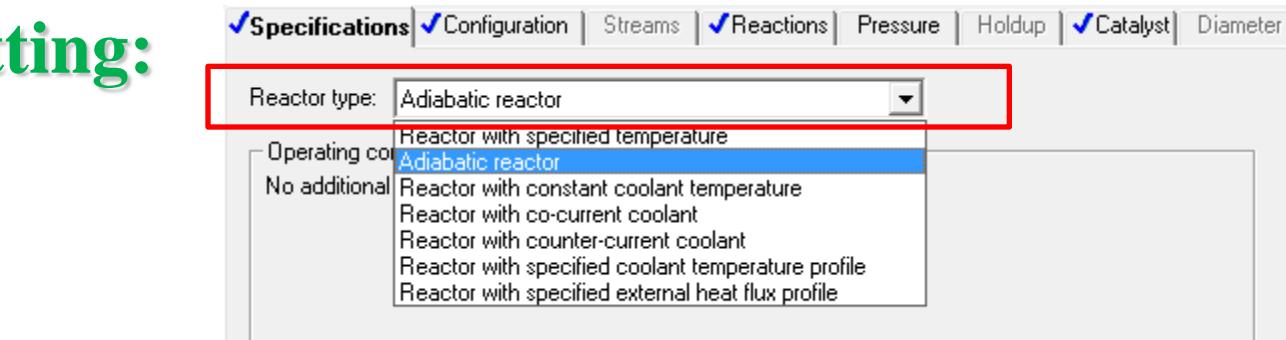
Power Law kinetic expression
Kinetic factor = $k(T/T_0)^n e^{-E/R(1/T - 1/T_0)}$

k:	3929.1	
n:	0	
E:	85458	kJ/kmol
T ₀ :		K
[C _i] basis:	Mole fraction	

Edit reactions Solids

KINETICS REACTORS: RPLUG

RPLUG Setting:



KINETICS REACTORS: RPLUG

RPLUG Setting:

The screenshot shows a software interface for process modeling. At the top, there is a navigation bar with several tabs: Specifications, Configuration, Streams, Reactions (which is highlighted with a blue checkmark), Pressure, Holdup, Catalyst, and Diameter. Below the navigation bar, there is a section titled "Select reaction set(s) to be included in the model". This section is divided into two columns: "Available reaction sets" and "Selected reaction sets". The "Available reaction sets" column is currently empty. The "Selected reaction sets" column contains one item, "R-1", which is highlighted with a red border. To the right of the "Selected reaction sets" column are four small buttons with arrows pointing in various directions (>, >>, <, <<).

KINETICS REACTORS: RPLUG

RPLUG Setting:

The screenshot shows the 'Catalyst' tab selected in the top navigation bar. A red box highlights the 'Catalyst present in reactor?' checkbox and the 'Ignore catalyst volume in rate/residence time calculations' checkbox. Below these, under 'Specifications', there are two input fields: 'Catalyst loading' set to 0.1865 kg and 'Bed voidage' set to 0.8928.

Catalyst loading	0.1865	kg
Bed voidage	0.8928	

Below the specifications, there is a section for 'Particle geometry' with 'Diameter' set to 0.328084 ft and 'Sphericity' set to 1.

Diameter:	0.328084	ft
Sphericity:	1	

Check result

Material			
Display: Streams Format: GEN_E Stream Table			
	FEED	PROD	
Temperature K	300.0	300.0	
Pressure atm	31.98	31.98	
Vapor Frac	1.000	1.000	
Mole Flow kmol/hr	1000.000	523.000	
Mass Flow kg/hr	9826.426	9826.426	
Volume Flow l/min	12981.346	4727.868	
Enthalpy MMBtu/hr	-38.969	-86.434	
Mole Flow kmol/hr			
CO	236.800	TRACE	
H2O	0.100	240.300	
CO2	36.100	34.400	
H2	717.200	0.001	
CH4	9.800	248.300	
Mole Frac			
CO	0.237	TRACE	
H2O	100 PPM	0.459	
CO2	0.036	0.066	
H2	0.717	1 PPM	
CH4	0.010	0.475	

Check result

The screenshot shows the Aspen Plus interface with the 'Process Stream' tab selected. On the left, a tree view of the project structure is shown, with 'B2' expanded to show various sub-options. The 'Profiles' option under 'B2' is highlighted with a red box. The main window displays a table of reactor profiles. The columns are labeled: Reactor length (meter), Pressure (N/sqm), Temperature (K), Molar vapor fraction, Duty (Watt), Residence time (sec), and Liquid holdup. The table contains 11 rows, each corresponding to a reactor length from 0 to 10 meters. The temperature column is highlighted with a red box.

Reactor length meter	Pressure N/sqm	Temperature K	Molar vapor fraction	Duty Watt	Residence time sec	Liquid holdup
0	100000	583	1	0	0	0
1	100000	592.302094	1	0	6455.72357	0
2	100000	598.56837	1	0	12828.0469	1.5686E-16
3	100000	602.399039	1	0	19147.0991	1.5586E-16
4	100000	604.575208	1	0	25434.6255	0
5	100000	605.76972	1	0	31705.0267	0
6	100000	606.414471	1	0	37966.2727	0
7	100000	606.758738	1	0	44222.6183	0
8	100000	606.942874	1	0	50476.3821	0
9	100000	607.041101	1	0	56728.7636	0
10	100000	607.093025	1	0	62980.4029	0

Check result

Select Reactor Length column



Plot -> x-Axis variable



Select Temperature Column



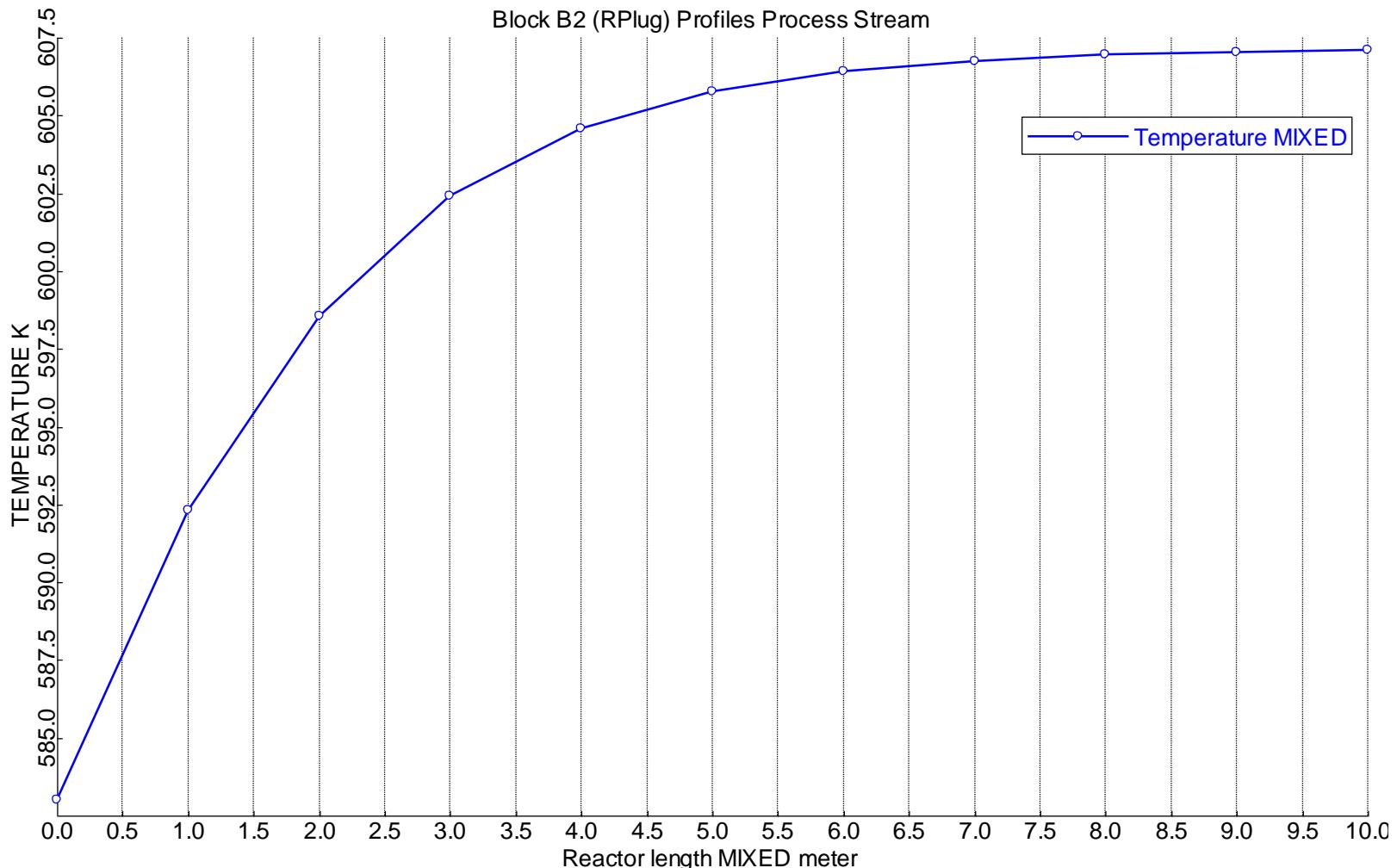
Plot -> y-Axis variable



Display Plot

Process Stream		Coolant Stream	Properties	User Variables	Component Attr.	PSD
Process stream profiles						
View:	Summary	Substream:	MIXED			
Reactor length	Pressure	Temperature	Molar vapor fraction	Duty	Residence time	Liquid holdup
meter	N/sqm	K		Watt	sec	
0	100000	583	1	0	0	0
1	100000	592.302094	1	0	6455.72357	0
2	100000	598.56837	1	0	12828.0469	1.5686E-16
3	100000	602.399039	1	0	19147.0991	1.5586E-16
4	100000	604.575208	1	0	25434.6255	0
5	100000	605.76972	1	0	31705.0267	0
6	100000	606.414471	1	0	37966.2727	0
7	100000	606.758738	1	0	44222.6183	0
8	100000	606.942874	1	0	50476.3821	0
9	100000	607.041101	1	0	56728.7636	0
10	100000	607.093025	1	0	62980.4029	0

Check result



Check result

The screenshot shows the Aspen Plus interface with the following details:

- Left Panel (Tree View):** Shows various project settings and configurations. A red box highlights the "Profiles" option under the "B2" block.
- Top Bar:** Contains tabs for "Process Stream", "Coolant Stream", "Properties", "User Variables", and "Compo".
- Sub-Panel:** Titled "Process stream profiles". It includes dropdown menus for "View: Molar composition" and "Substream: MIXED".
- Table:** Displays molar composition data for a process stream. The columns are Length (meter), CO, H₂O, CO₂, and H₂. The rows show values from 0 to 10 meters.

Length meter	CO	H ₂ O	CO ₂	H ₂
0	0.03	0.392	0.148	0.43
1	0.02171766	0.38371767	0.15628233	0.43828233
2	0.01610643	0.37810644	0.16189356	0.44389356
3	0.01266345	0.37466345	0.16533655	0.44733655
4	0.01070319	0.37270319	0.16729681	0.44929681
5	0.00962585	0.37162586	0.16837415	0.45037415
6	0.00904395	0.37104396	0.16895604	0.45095604
7	0.00873313	0.37073314	0.16926686	0.45126686
8	0.00856685	0.37056686	0.16943314	0.45143314
9	0.00847814	0.37047815	0.16952185	0.45152185
10	0.00843125	0.37043125	0.16956875	0.45156875

Check result

Select Reactor Length column



Plot -> x-Axis variable



Select all other columns



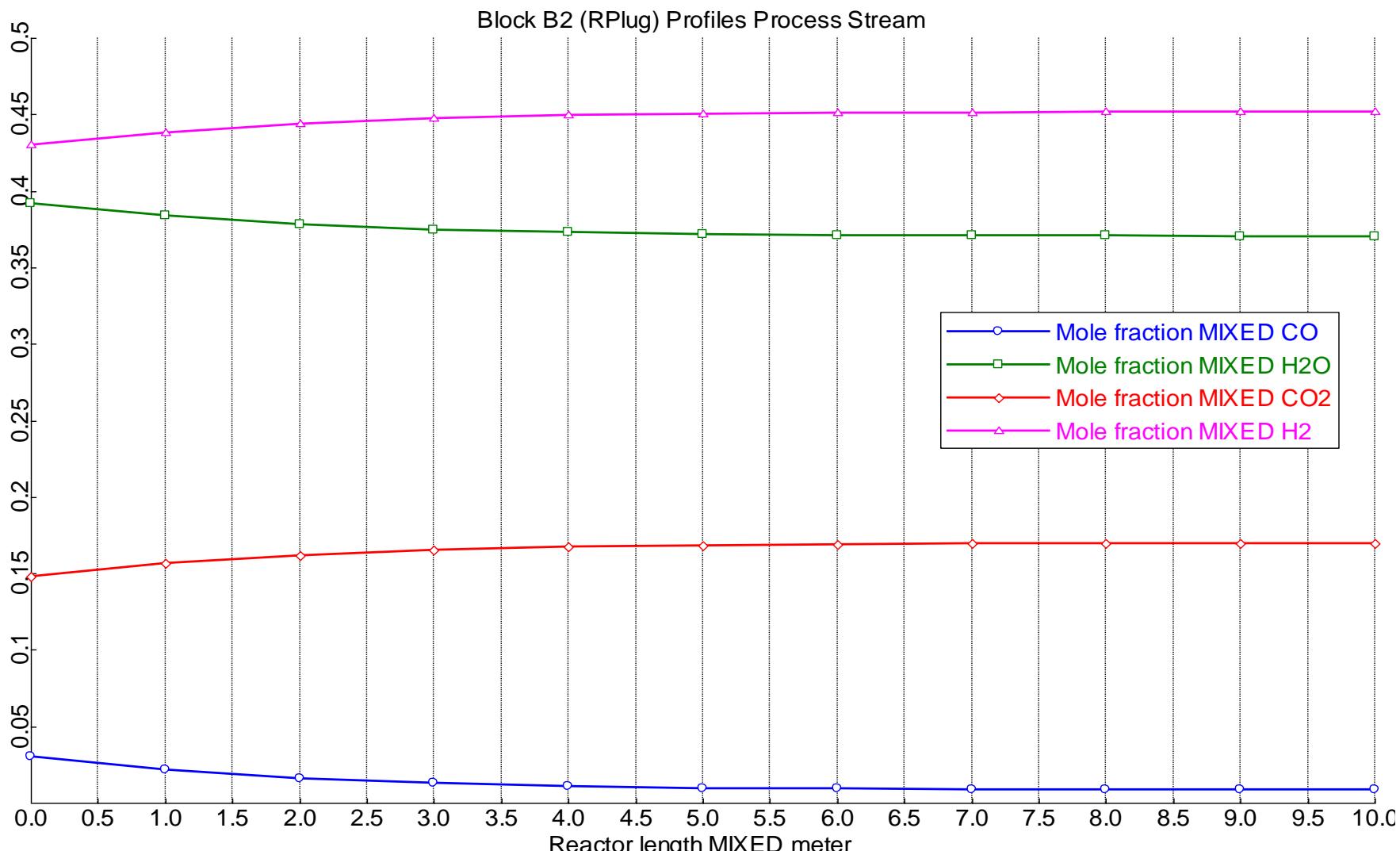
Plot -> y-Axis variable



Display Plot

Process Stream		Coolant Stream	Properties	User Variables	Compo
Process stream profiles					
View:	Molar composition	Substream:	MIXED		
Length	CO	H2O	CO2	H2	
meter					
0	0.03	0.392	0.148	0.43	
1	0.02171766	0.38371767	0.15628233	0.43828233	
2	0.01610643	0.37810644	0.16189356	0.44389356	
3	0.01266345	0.37466345	0.16533655	0.44733655	
4	0.01070319	0.37270319	0.16729681	0.44929681	
5	0.00962585	0.37162586	0.16837415	0.45037415	
6	0.00904395	0.37104396	0.16895604	0.45095604	
7	0.00873313	0.37073314	0.16926686	0.45126686	
8	0.00856685	0.37056686	0.16943314	0.45143314	
9	0.00847814	0.37047815	0.16952185	0.45152185	
10	0.00843125	0.37043125	0.16956875	0.45156875	

Check result



KINETICS REACTORS: RCSTR

Reaction :Exothermic & Irreversible

Aniline + Hydrogen → Cyclohexylamine (CHA)

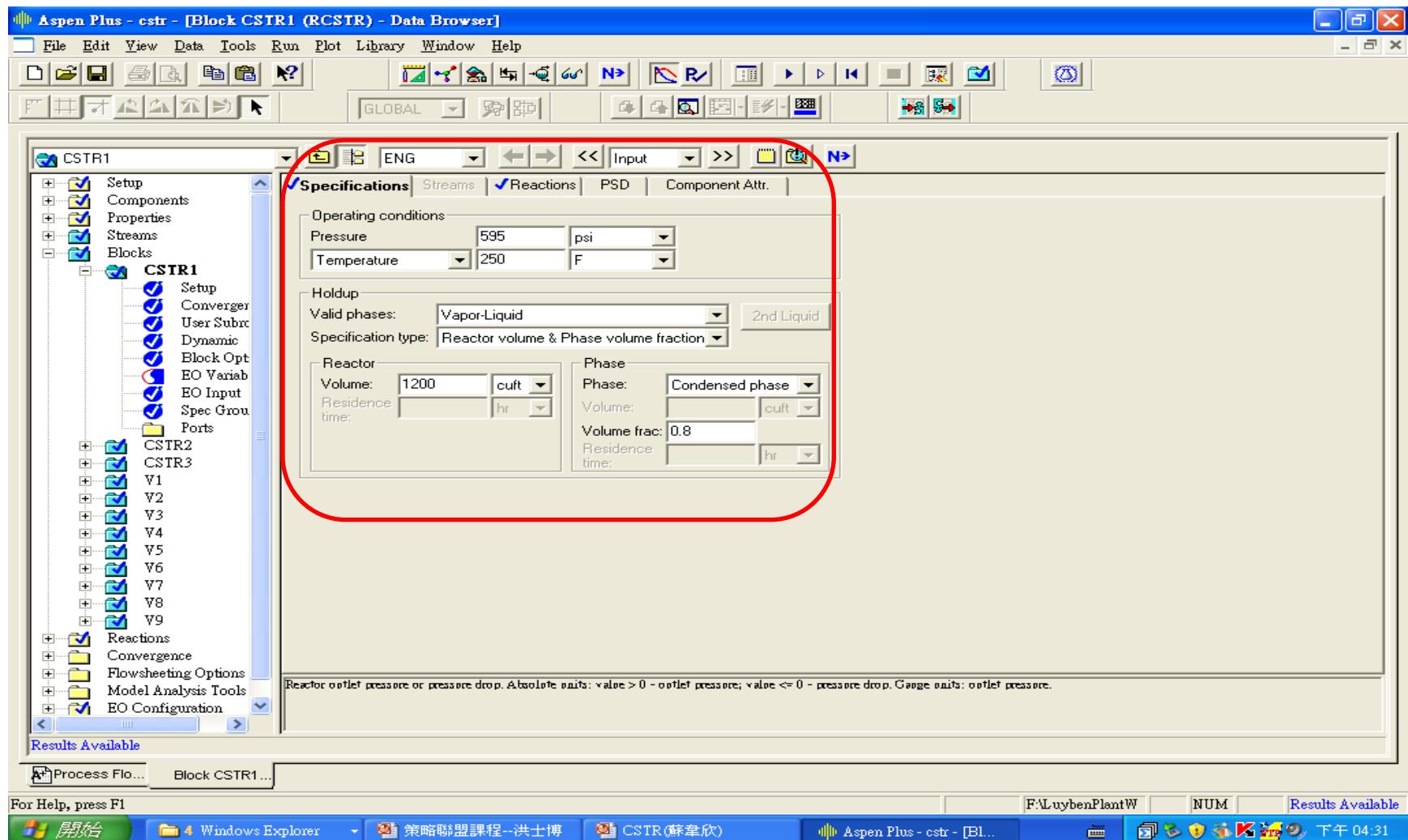


Reactor Conditions

Reactor :

Reactor condition	Pressure	595 psi
	Temperature	250 F
	Volume	1200 ft ³
Reactor type	Vertical cylindrical vessel	
Reactor liquid level	80%	

Reactor Conditions Input



Reaction Kinetics

Reaction rate :

$$R_{CHA} = kV_R C_A C_H$$

Where

V_R : reactor volume

C_A : concentration of Aniline

C_H : concentration of Hydrogen

• **Reaction kinetics :**

$$k = k_0 \exp(-E/RT)$$

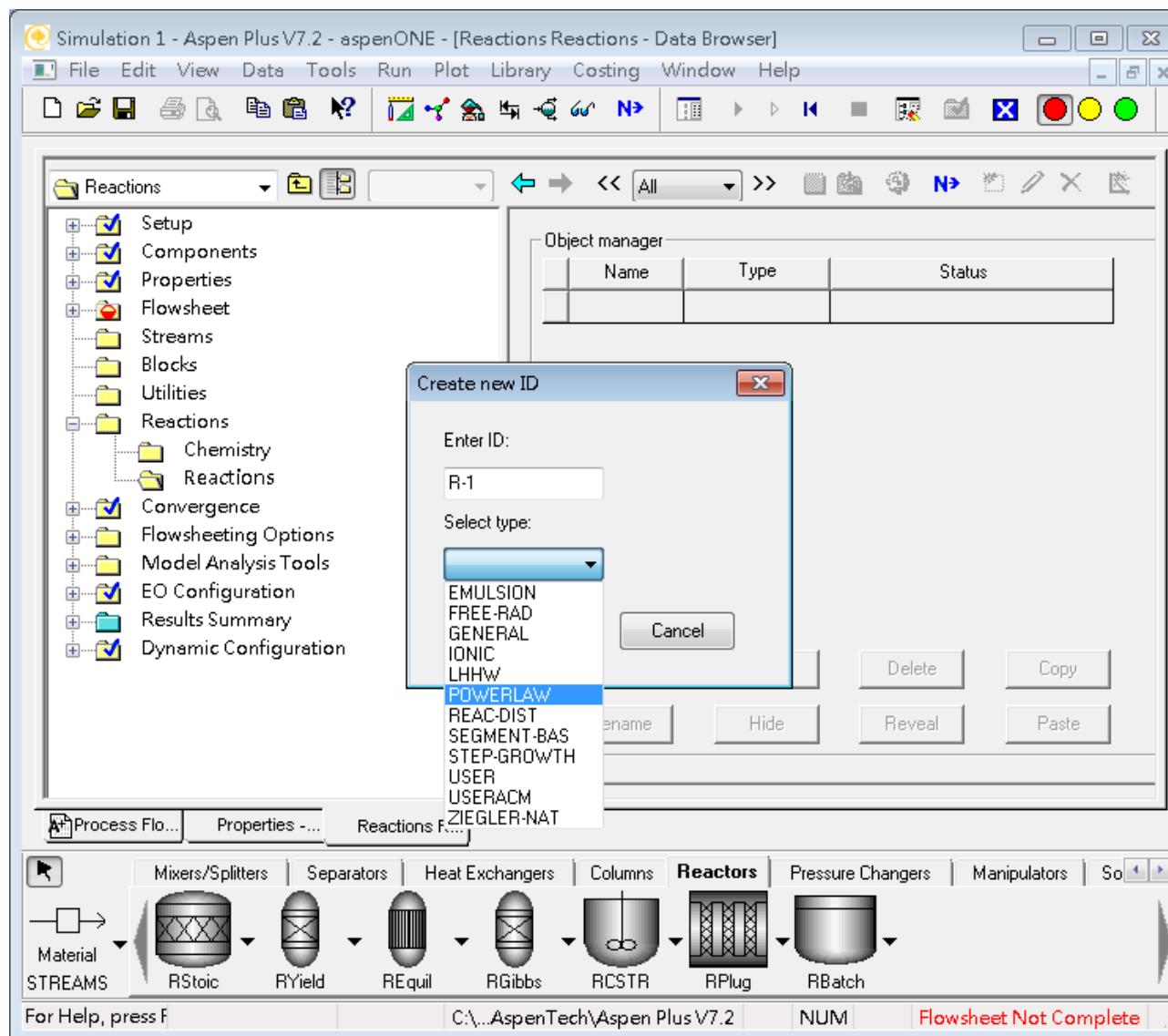
Where

T : temperature (R)

E : activity energy

$$E = 2000 \text{ Btu/lbmole}$$

Reaction Kinetics Input



Reaction Kinetics Input

The screenshot shows the Aspen Plus V7.2 interface with the title bar "Simulation 1 - Aspen Plus V7.2 - aspenONE - [Reactions Reactions R-1 (POWERLAW) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The main workspace displays a tree view under "R-1" with checked nodes for Components, Properties, Flowsheet, Streams, and Blocks. A sub-node "B1" is expanded, showing a "Setup" folder. To the right, a tab bar has "Stoichiometry" selected, along with Kinetic, Equilibrium, and Activity tabs. Below this is a table:

Rxn No.	Reaction type	Stoichiometry
1	Kinetic	ANILI-01 + 3 HYDRO-01 → CYCLO-01

A dialog box titled "Edit Reaction" is open in the foreground. It contains fields for "Reaction No.: 1" and "Reaction type: Kinetic". The "Reactants" section shows the following table:

Component	Coefficient	Exponent
ANILI-01	-1	1
HYDRO-01	-3	1
*		

The "Products" section shows the following table:

Component	Coefficient	Exponent
CYCLO-01	1	
*		

At the bottom of the dialog are "N>" and "Close" buttons. The bottom navigation bar includes buttons for RStoic, RYield, REquil, RGibbs, RCSTR, RPlug, and RBatch, with "RStoic" currently highlighted. The status bar at the bottom displays "For Help, press F1", the path "C:\...AspenTech\Aspen Plus V7.2", and "Required Input Complete".

Reaction Kinetics Input

Simulation 1 - Aspen Plus V7.2 - aspenONE - [Reactions Reactions R-1 (POWERLAW) - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

R-1 ENG

Stoichiometry Kinetic Equilibrium Activity

1) ANILI-01 + 3 HYDRO-01 → CYCLO-01

Reacting phase: Liquid Rate basis: Rec (vol)

Power Law kinetic expression
Kinetic factor = $k(T/T_0)^n e^{-E/R}(1/T - 1/T_0)$

k: 1750
n: 0
E: 11111 cal/mol
T₀: F
[C] basis: Molarity

Edit reactions Solids

Process Flow Control Panel Properties Stream 2 (M...) Reactions R...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators So

Material STREAMS RStaic RYield REquil RGibbs RCSTR RPlug RBatch

C:\...AspenTech\Aspen Plus V7.2 NUM Required Input Complete

Feeds Conditions

Two fresh feed stream :

	Aniline feed	Hydrogen feed
mole rate	100 lbmolhr^{-1}	400 lbmolhr^{-1}
temperature	100 F	100 F
pressure	650 psia	650 psia

Feeds Conditions

Specifications Flash Options PSD Component Attr. EO Options

Substream name: **MIXED** Ref Temperature

State variables

Temperature	100	F
Pressure	650	psia

Total flow: Mole lbmol/hr

Solvent:

Composition

Mole-Flow	lbmol/hr
Component	Value
ANILI-01	100
HYDRO-01	
CYCLO-01	

Total: 100

Specifications Flash Options PSD Component Attr. EO Options

Substream name: **MIXED** Ref Temperature

State variables

Temperature	100	F
Pressure	650	psia

Total flow: Mole lbmol/hr

Solvent:

Composition

Mole-Flow	lbmol/hr
Component	Value
ANILI-01	
HYDRO-01	400
CYCLO-01	

Total: 400

Check result

		1	2	3	
Substream: MIXED					
Mole Flow lbmol/hr					
ANILI-01	100.0000	0.0	23.63094		
HYDRO-01	0.0	400.0000	170.8928		
CYCLO-01	0.0	0.0	76.36906		
Mole Frac					
ANILI-01	1.000000	0.0	.0872335		
HYDRO-01	0.0	1.000000	.6308503		
CYCLO-01	0.0	0.0	.2819162		
Total Flow lbmol/hr	100.0000	400.0000	270.8928		
Total Flow lb/hr	9312.832	806.3520	10119.18		
Total Flow cuft/hr	147.8783	3794.312	2436.992		
Temperature F	100.0000	100.0000	250.0000		
Pressure psia	650.0000	650.0000	595.0000		
Vapor Frac	0.0	1.000000	.6354694		
Liquid Frac	1.000000	0.0	.3645306		

Question:

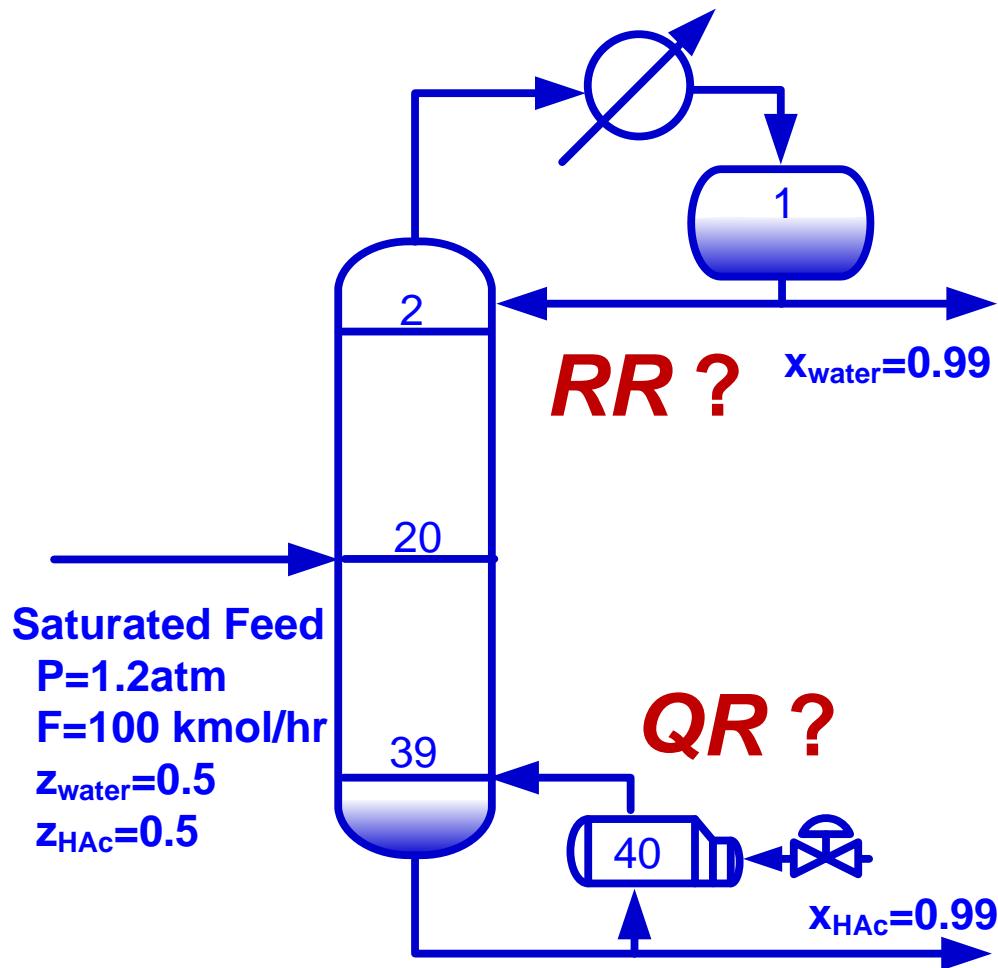
- (1) Compare the conversion between RSTOIC and RCSTR.
- (2) Compare the net duty inside the RSTOIC and RCSTR

Introduction to Aspen Plus

Part 6: Running simulation

Distillation Process (DSTWU, RADFRAC)

Distillation Separation



- There are two degrees of freedom to manipulate distillate composition and bottoms composition to manipulate the distillate and bottoms compositions.
- If the feed condition and the number of stages are given, how much of RR and QR are required to achieve the specification.

Distillation Separation

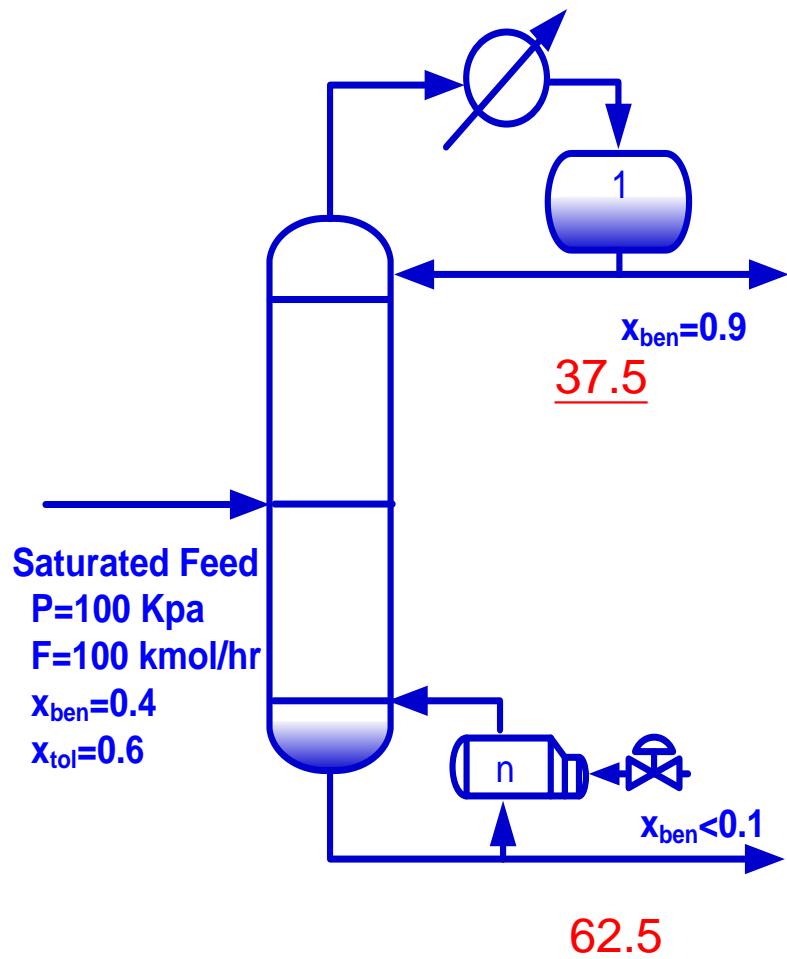
Example :

A mixture of benzene and toluene containing 40 mol% benzene is to be separated to give a product containing 90 mol% benzene at the top, and no more than 10% benzene in bottom product. The feed enters the column as saturated liquid, and the vapor leaving the column which is condensed but not cooled, provide reflux and product. It is proposed to operate the unit with a reflux ratio of 3 kmol/kmol product. Please find:

- (1) The number of theoretical plates.
- (2) The position of the entry.

(Problem is taken from Coulson & Richardson's Chemical Engineering, vol 2, Ex 11.7, p.564)

1. By what you learned in Material balance and unit operation



From Overall Material Balance:

$$100 = D + B$$

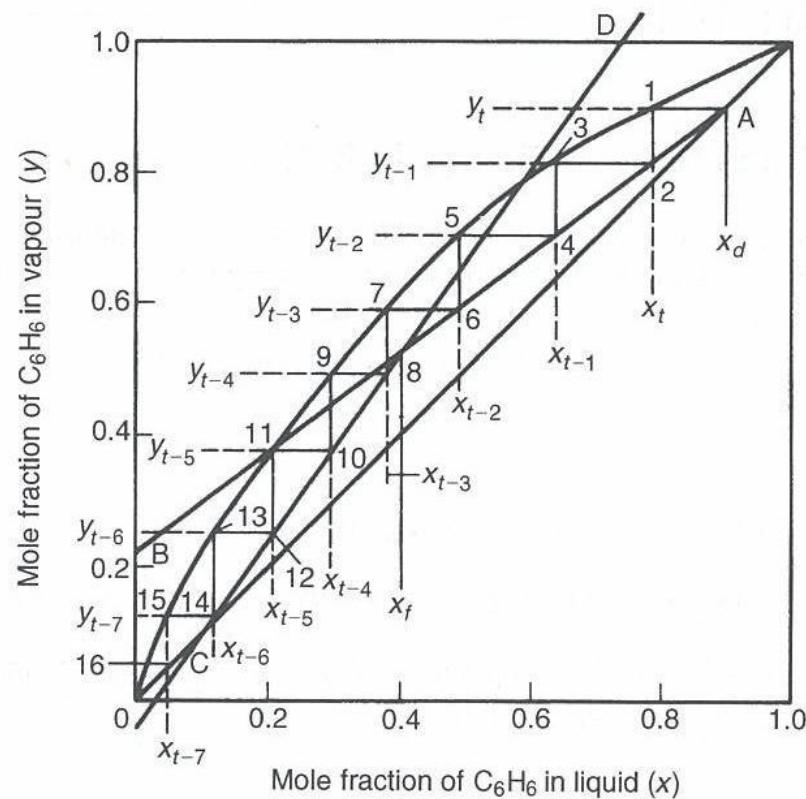
From Benzene Balance:

$$100 * 0.4 = 0.9 * D + 0.1 * B$$

Thus, D=37.5 and B=62.5.

1. By what you learned in Material balance and unit operation

From thermodynamic phase equilibrium, and the calculation of operating line:



Solution

a) From a material balance for a feed of 100 kmol:

$$V_n = V_m = 150; L_n = 112.5; L_m = 212.5; D = 37.5 \text{ and } W = 62.5 \text{ kmol}$$

b) The equilibrium curve and the diagonal line are drawn in as shown in Figure 11.15.

c) The equation of the top operating line is:

$$y_n = 0.75x_{n+1} + 0.225$$

Thus, the line AB is drawn through the two points A (0.9, 0.9) and B (0, 0.225).

d) The equation of the bottom operating line is:

$$y_m = 1.415x_{m+1} - 0.042 \quad (\text{ii})$$

This equation is represented by the line CD drawn through C (0.1, 0.1) at a slope of 1.415.

e) Starting at point A, the horizontal line is drawn to cut the equilibrium line at point 1. The vertical line is dropped through 1 to the operating line at point 2 and this procedure is repeated to obtain points 3–6.

f) A horizontal line is drawn through point 6 to cut the equilibrium line at point 7 and a vertical line is drawn through point 7 to the lower enrichment line at point 8. This procedure is repeated in order to obtain points 9–16.

g) The number of stages are then counted, that is points 2, 4, 6, 8, 10, 12, and 14 which gives the number of plates required as 7.

We can get the number of theoretical plate to be 7.

2. By the shortcut method in Aspen Plus (DISTWU) (Add components)

The screenshot shows the Aspen Plus V7.2 interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Components Specifications - Data Browser]". The left sidebar has a tree view with checked items: Setup, Components (Specifications, Assay/Blend, Light-End Properties, Petro Characterization, Pseudocomponents, Attr-Comps, Henry Comps, Moisture Comps, UNIFAC Groups, Comp-Groups, Comp-Lists, Polymers, Attr-Scaling), Properties, Flowsheet, Streams, Blocks, Utilities, Reactions, Convergence, and Flowsheeting Options. The main area shows a "Selection" tab with "Petroleum" and "Nonconventional" selected, and "Enterprise Database" checked. A table titled "Define components" lists components: BEN (Conventional, BENZENE, C6H6) and TOL (Conventional, TOLUENE, C7H8). An asterisk (*) row is also present. Below the table are buttons: Find (circled in blue), Elec Wizard, User Defined, Reorder, and Review. A red box highlights the table area. A blue arrow points from the "Find" button towards the table. Red text "Built in the components" is overlaid on the right side of the table area. The bottom toolbar includes icons for Material STREAMS, Mixers/Splitters (DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, BatchSep), Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The status bar at the bottom shows "For Help, press F1", "C:\...AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

Component ID	Type	Component name	Formula
BEN	Conventional	BENZENE	C6H6
TOL	Conventional	TOLUENE	C7H8
*			

Built in the components

2. By the shortcut method in Aspen Plus (DISTWU) (Select property method)

The screenshot shows the Aspen Plus V7.2 Properties - Data Browser window. On the left, a tree view under 'Properties' shows various categories like Assay/Blend, Light-End Properties, Petro Characterization, etc., with 'Properties' selected and highlighted by a red box. On the right, the 'Global' tab is active, displaying property method settings. A red box highlights the 'Base method' dropdown, which is set to 'NRTL'. Below it, the 'Property method' dropdown is also set to 'NRTL'. A large red text overlay 'Select NRTL' is centered over the property method section. At the bottom, there's a note: 'Commonly used property methods. Use the Property Method Selection Assistant for help.'

Simu1 - Aspen Plus V7.2 - aspenONE - [Properties - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Properties

Assay/Blend
Light-End Properties
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
Moisture Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Polymers
Attr-Scaling
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Data
Analysis
Prop-Sets
Advanced
CAPE-OPEN Packages

Input Complete

Process Flow Properties - ...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS

DSTWU Dist RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...AspenTech\Aspen Plus V7.2 NUM Input Changed

2. By the shortcut method in Aspen Plus (DISTWU) (Select property method)

The screenshot shows the Aspen Plus V7.2 Data Browser interface. On the left, the navigation tree under 'NRTL-1' is expanded, with several nodes highlighted by red boxes:

- Properties
- Parameters
- NRTL-1 (highlighted)

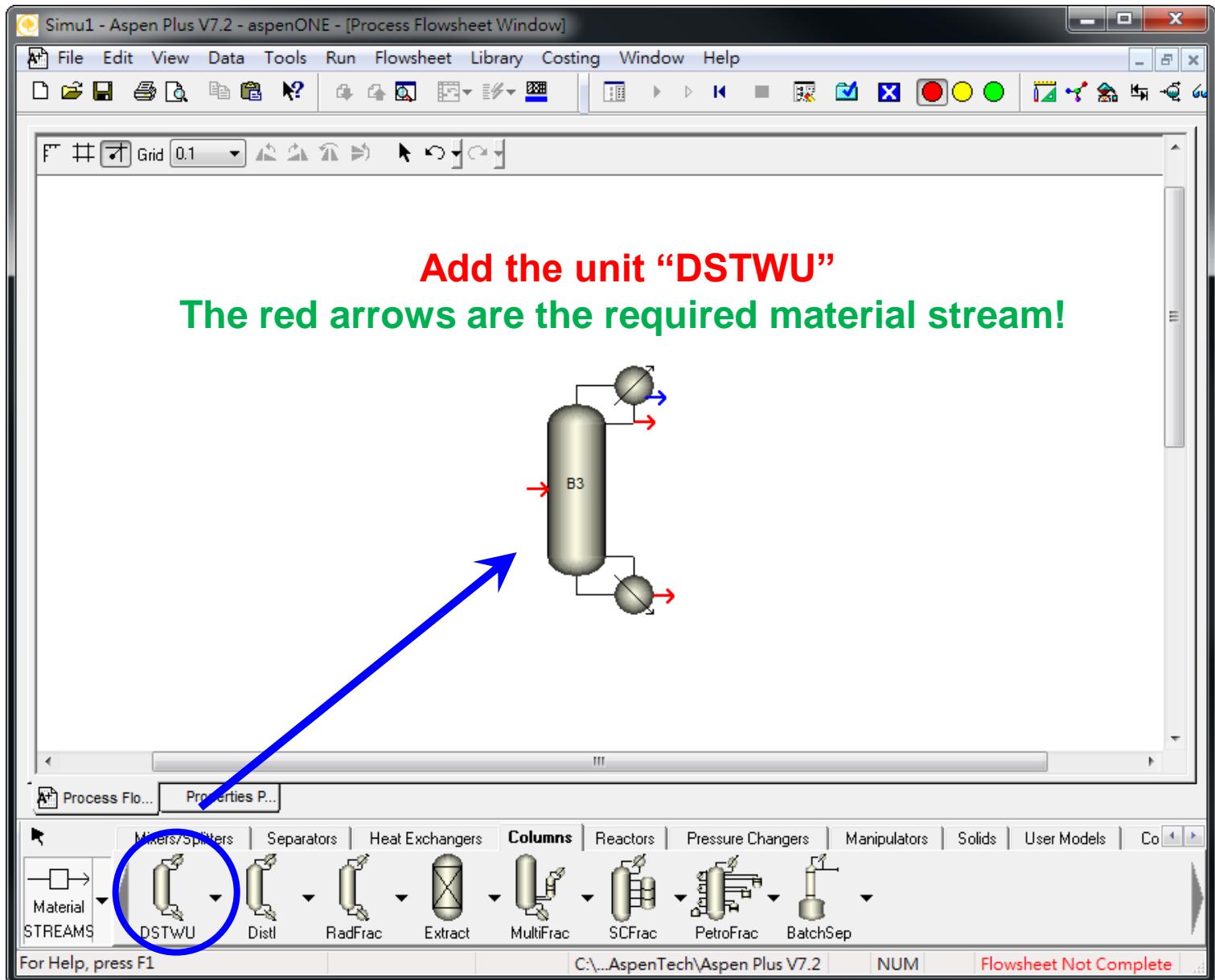
The main panel displays the 'Input' tab for 'NRTL'. It includes fields for 'Parameter' (set to 'NRTL') and 'Data set' (set to '1'). A table titled 'Temperature-dependent binary parameters' lists values for components BEN and TOL at temperature units K. The table also includes columns for AIJ, AJI, BIJ, and BJI.

	Component i	Component j
Temperature units	K	
Source	APV72 VLE-IG	
Property units:		
AIJ	-2.885200000	
AJI	2.191100000	
BIJ	1123.950100	
BJI	-863.7308000	

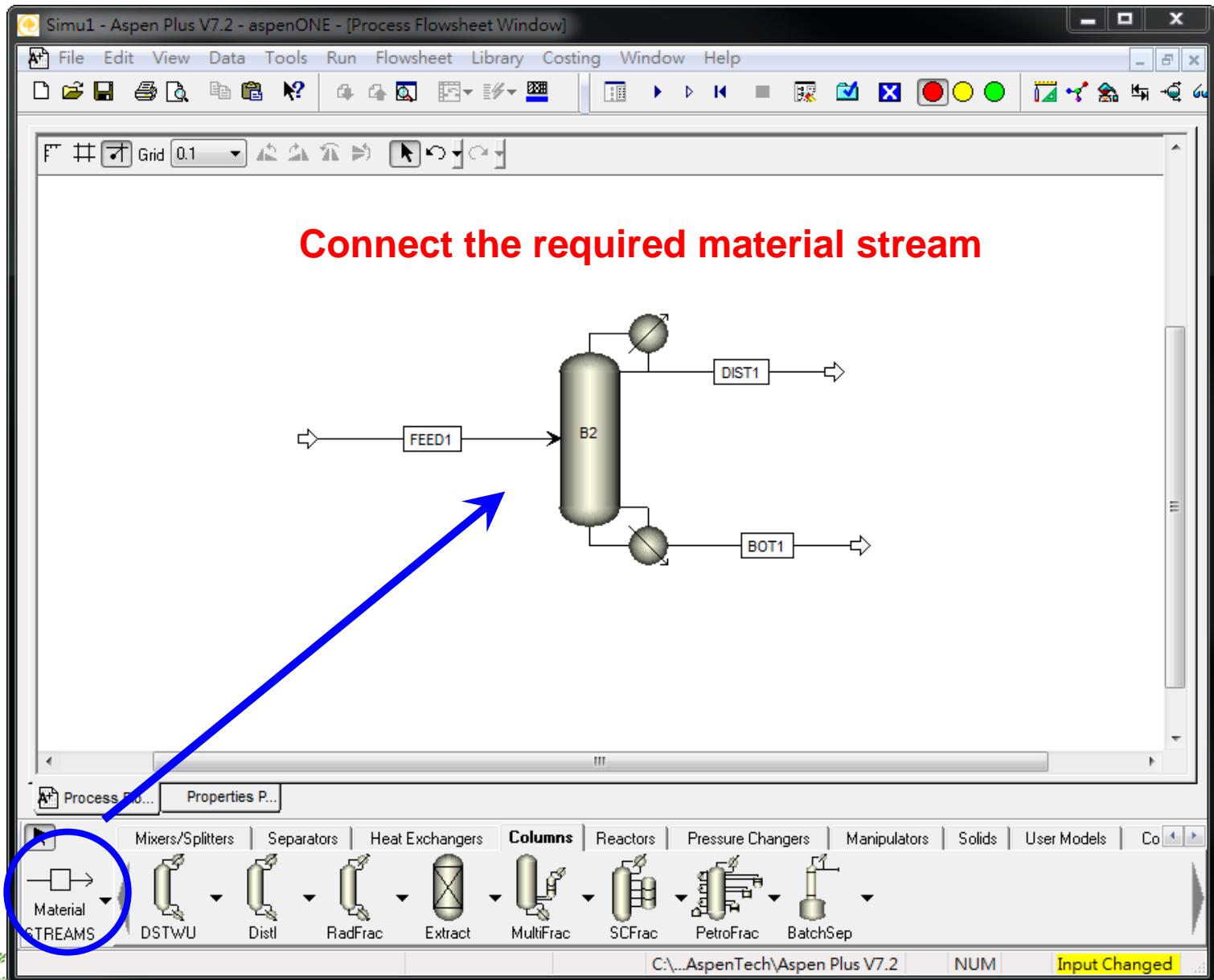
A red box highlights the text 'Check the binary parameters'.

At the bottom, there are tabs for 'Process Flow' and 'Properties P...', and a toolbar with various process equipment icons like Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co.

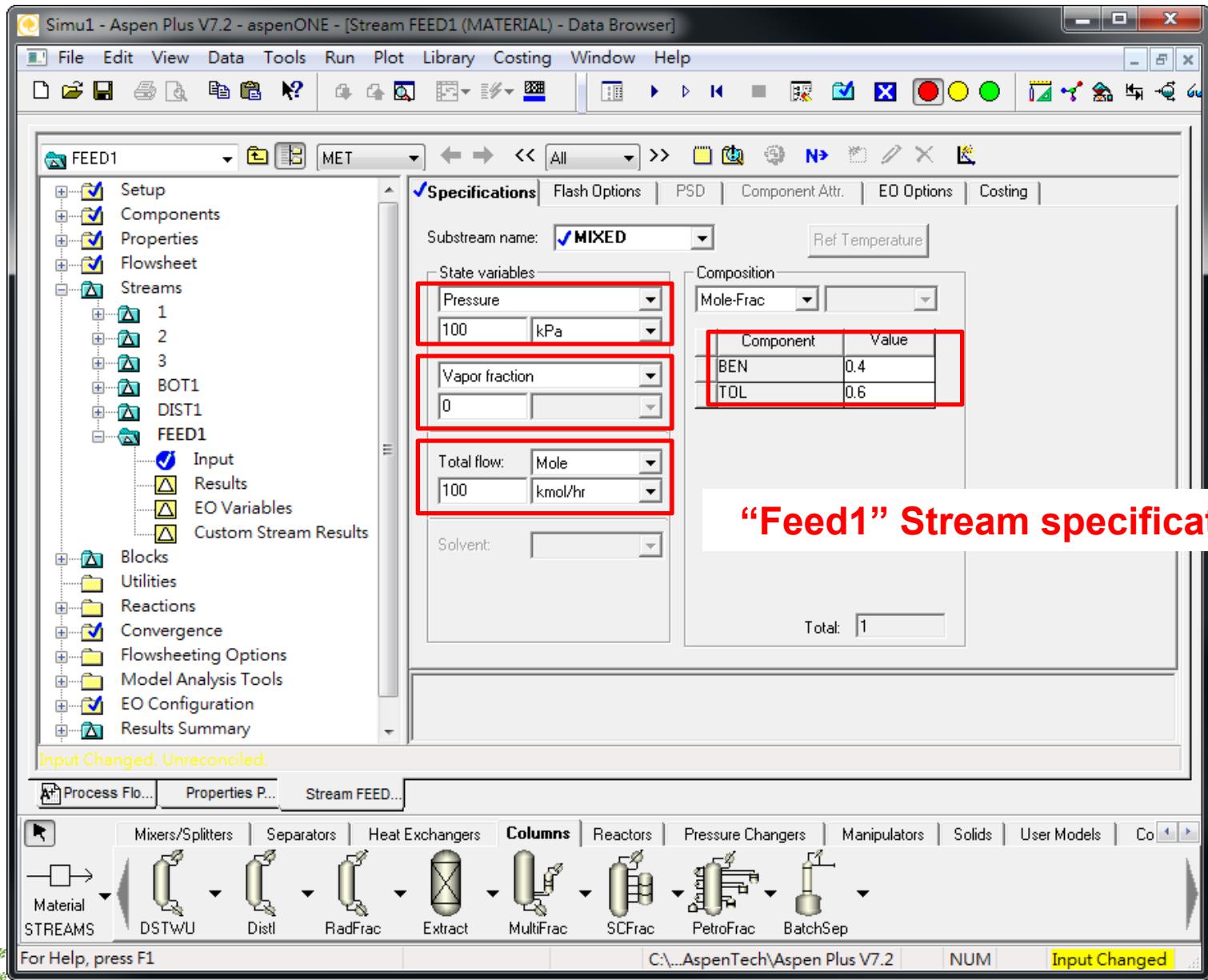
2. By the shortcut method in Aspen Plus (DSTWU)



2. By the shortcut method in Aspen Plus (DSTWU)



2. By the shortcut method in Aspen Plus (DSTWU)



2. By the shortcut method in Aspen Plus (Column Specification)

The screenshot shows the Aspen Plus V7.2 software interface. The main window title is "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B2 (DSTWU) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, Help. The toolbar has various icons for file operations. The left sidebar tree view shows "B2" selected, with branches for Setup, Components, Properties, Flowsheet, Streams, and Blocks (including B1 and B2). The "Blocks" section is expanded, showing Input, Block Options, Results, EO Variables, EO Input, Spec Groups, Ports, Stream Results, and Custom Stream Results. The "Utilities" section is also expanded, showing Reactions, Convergence, Flowsheeting Options, Model Analysis Tools, and EO Configuration. A message "Input Changed" is displayed at the bottom of the sidebar.

The central workspace displays the "Specifications" tab of the "Block B2 (DSTWU)" dialog. The "Column specifications" section contains two radio buttons: "Number of stages:" (set to 7) and "Reflux ratio:" (set to 3, highlighted with a red box). The "Pressure" section contains three input fields: "Condenser: 100 kPa" and "Reboiler: 100 kPa" (both highlighted with a red box), and a note below stating "Molar reflux ratio, if greater than 0, desired reflux ratio; if less than -1, desired reflux ratio is specified value times the minimum reflux ratio." Below the dialog, a message "From the problem" is displayed above the column specification parameters, and another message "Assume no pressure drop Inside the column" is displayed below the pressure settings.

At the bottom, a toolbar shows icons for Process Flow, Properties P..., Stream FEE..., and Block B2 (D...). The main toolbar includes Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep. The status bar at the bottom shows "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

2. By the shortcut method in Aspen Plus (Column Specification)

The screenshot shows the Aspen Plus V7.2 interface. The left sidebar displays the project structure under 'B2' with various blocks like B1 and B2 selected. The main window shows the 'Specifications' tab of the 'Block B2 (DSTWU)' dialog. Key parameters visible include:

- Column specifications:** Reflux ratio set to 3.
- Pressure:** Condenser at 100 kPa, Reboiler at 100 kPa.
- Key component recoveries:** Light key component BEN with recovery of 0.84375, highlighted with a red box.
- Condenser specifications:** Total condenser selected.
- Distillate vapor fraction:** Set to 0.

A large blue arrow points from the text 'Light Key recovery' to the 'Recov' field for the light key component.

Light Key recovery
= (mol of light component in distillate) /
(mol of light component in feed)
= $(37.5 * 0.9) / (100 * 0.4)$
= 0.84375

2. By the shortcut method in Aspen Plus (Column Specification)

The screenshot shows the Aspen Plus V7.2 interface with the following details:

- Left Sidebar:** Shows the project structure under "B2" with nodes like Setup, Components, Properties, Flowsheet, Streams, and Blocks (B1, B2). B2 is expanded to show Input, Block Options, Results, EO Variables, EO Input, Spec Groups, Ports, Stream Results, and Custom Stream Results.
- Specifications Tab:** Under "MET", the "Specifications" tab is selected. It includes:
 - Column specifications:** Reflux ratio is set to 3.
 - Pressure:** Condenser pressure is 100 kPa, Reboiler pressure is 100 kPa.
 - Key component recoveries:**
 - Light key:** Component BEN, Recovery 0.84375.
 - Heavy key:** Component TOL, Recovery 0.0625 (highlighted with a red box).
 - Condenser specifications:** Total condenser is selected.
- Bottom Toolbar:** Shows icons for Process Flow, Properties, Stream FEE, and Block B2 (DSTWU). The DSTWU icon is highlighted.
- Bottom Panel:** Shows categories like Mixers/Splitters, Separators, Heat Exchangers, Columns, and various stream and separator components.

Calculation:

Heavy Key recovery

= (mol of heavy component in distillate) / (mol of heavy component in feed)

= $(37.5 * 0.1) / (100 * 0.6)$

= 0.0625

2. By the shortcut method in Aspen Plus (Column Specification)

The screenshot shows the Aspen Plus V7.2 Data Browser interface. On the left is a navigation tree with nodes like Setup, Components, Properties, Flowsheet, Streams, and Blocks (with B1 and B2 expanded). The right pane has tabs for Specifications, Calculation Options, and Convergence. The Specifications tab is active. A red box highlights the 'Options' section with checkboxes for 'Generate table of reflux ratio vs number of theoretical stages' (checked) and 'Calculate HETP' (unchecked). Another red box highlights the 'Table of actual reflux ratio vs number of theoretical stages' section, which includes fields for Initial number of stages (15), Final number of stages (6), Increment size for number of stages (1, selected), Number of values in table (11), and Significant digits displayed in table (5). A blue arrow points from this section to a text box below it that reads 'Increment size for number of stages.' A large blue text box on the right states: 'Get results by varying the number of stages. (Initial Guess)'.

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B2 (DSTWU) - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

B2

Setup Components Properties Flowsheet Streams Blocks B1 B2 Input Block Options Results EO Variables EO Input Spec Groups Ports Stream Results Custom Stream Results Utilities Reactions Convergence Flowsheeting Options Model Analysis Tools EO Configuration

Specifications Calculation Options Convergence

Options

Generate table of reflux ratio vs number of theoretical stages

Calculate HETP

Table of actual reflux ratio vs number of theoretical stages

Initial number of stages: 15

Final number of stages: 6

Increment size for number of stages: 1

Number of values in table: 11

Significant digits displayed in table: 5

HETP calculation

Packed height:

Increment size for number of stages.

Get results by varying the number of stages. (Initial Guess)

Input Changed

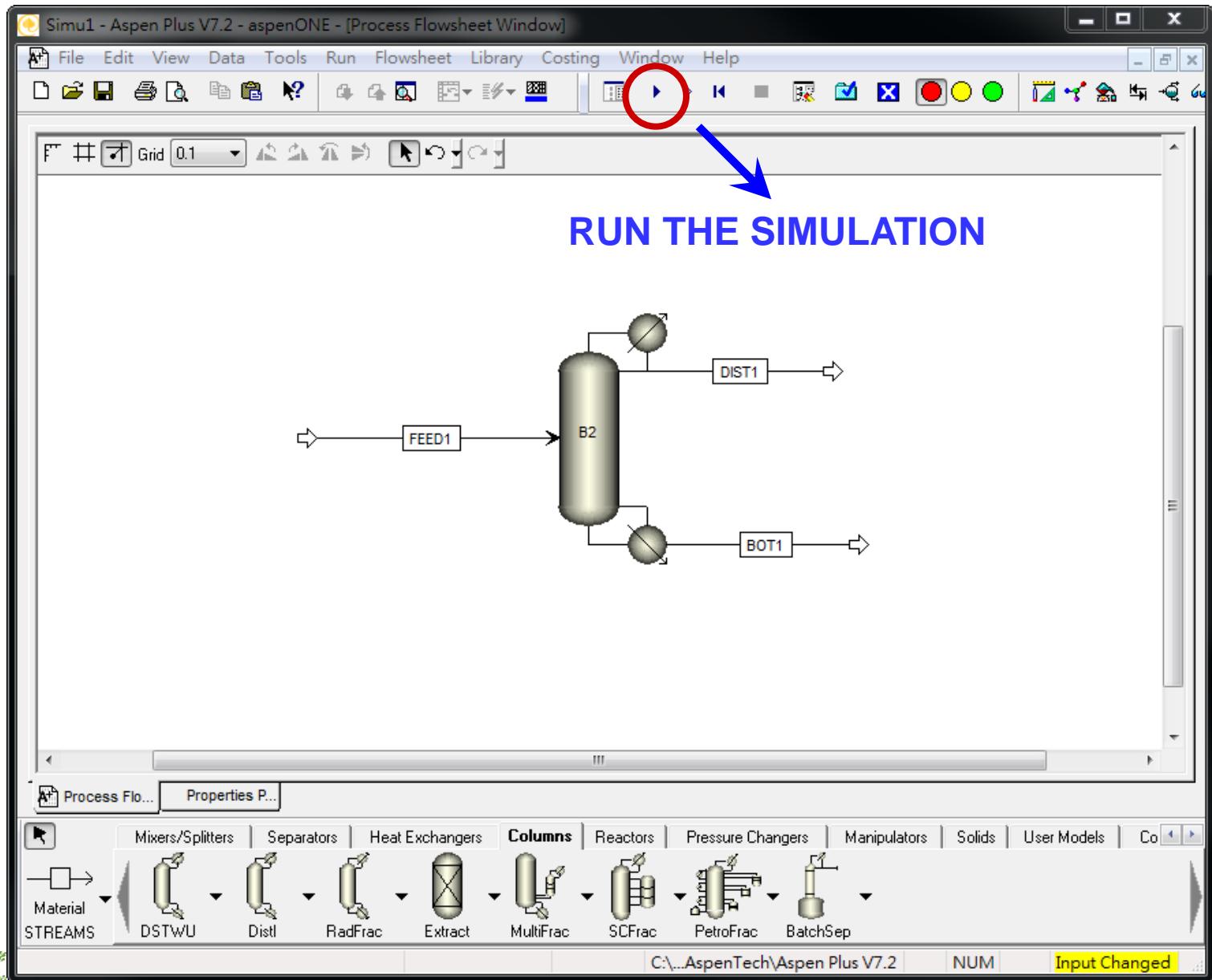
Process Flow... Properties P... Stream FEE... Block B2 (D...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co...

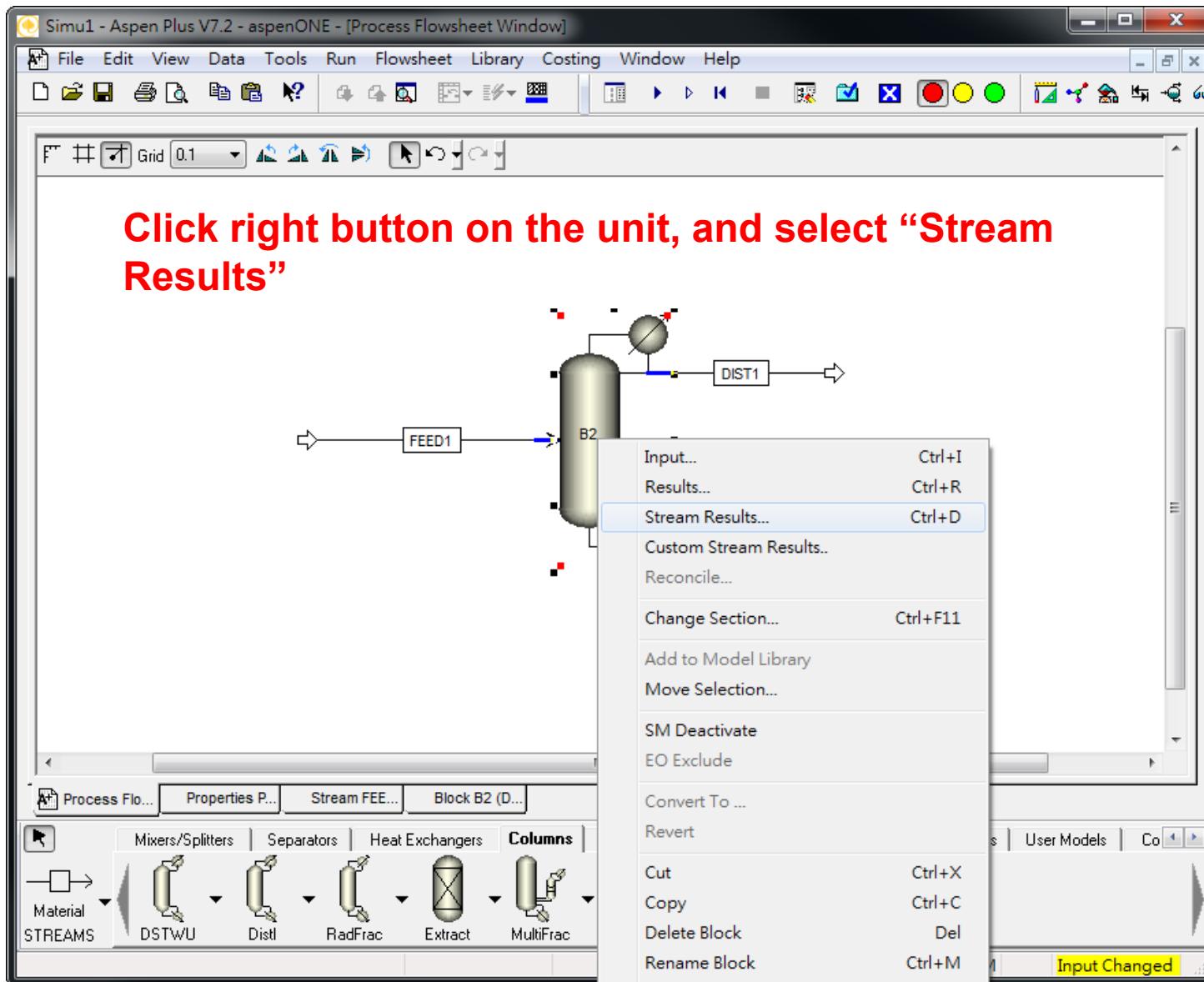
Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

2. By the shortcut method in Aspen Plus (DSTWU)



2. By the shortcut method in Aspen Plus (Stream Results)



2. By the shortcut method in Aspen Plus (Stream Results)

The screenshot shows the Aspen Plus V7.2 software interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B2 (DSTWU) Stream Results - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar shows the project structure under "Stream Results" with "Blocks" expanded to show B1 and B2, and "Results" expanded to show "Results", "EO Variables", "Stream Results", and "Custom Stream Results". Other sections include "EO Configuration" and "Results Summary". The main area is titled "Material" and displays a "Stream Table". The "Display" dropdown is set to "Streams" and the "Format" dropdown is set to "GEN_E". The table lists stream properties: Mass Flow kg/hr, Volume Flow l/min, Enthalpy MMBtu/hr, Mole Flow kmol/hr, BEN mole fraction, and TOL mole fraction. The bottom row shows the required product quality: BEN at 0.900 and TOL at 0.100, both highlighted with a red border. A message box at the bottom right says "The required product quality". The bottom navigation bar includes tabs for Process Flow, Properties P..., Stream FEE..., Block B2 (D...), and Block B2 (D...). The toolbar below the tabs includes icons for Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The bottom panel shows a library of process equipment: Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

	FEED1	DIST1	BOT1	
Mass Flow kg/hr	8652.977	2981.862	5671.114	
Volume Flow l/min	181.114	61.218	120.357	
Enthalpy MMBtu/hr	3.652	1.915	1.768	
Mole Flow kmol/hr				
BEN	40.000	33.750	6.250	
TOL	60.000	3.750	56.250	
Mole Frac				
BEN	0.400	0.900	0.100	
TOL	0.600	0.100	0.900	

The required product quality

Input Changed

Process Flow Properties P... Stream FEE... Block B2 (D...) Block B2 (D...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

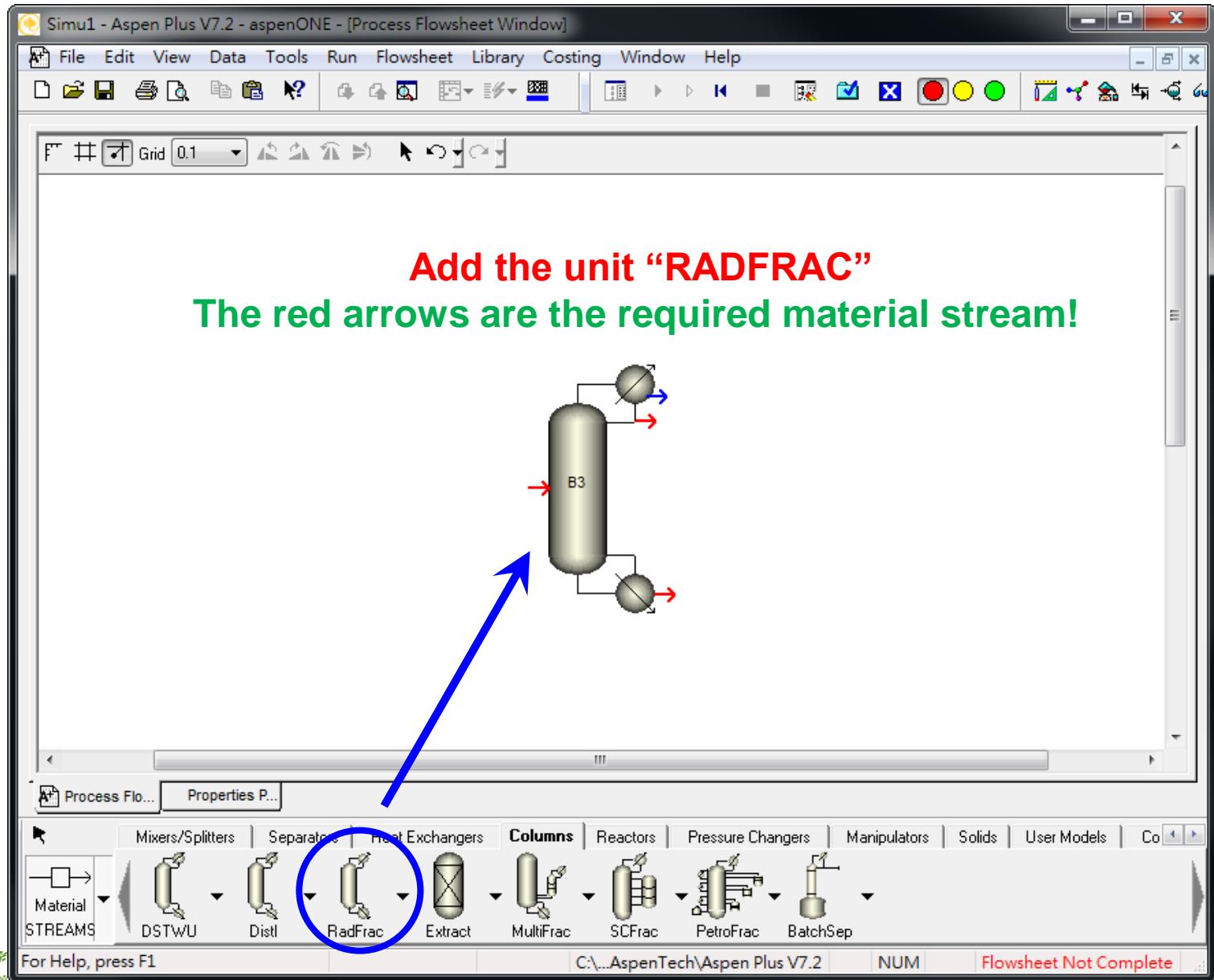
2. By the shortcut method in Aspen Plus (RR vs number of stage)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B2 (DSTWU) Results - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation controls. On the left, a tree view of the project structure is shown under "Results", including Setup, Components, Properties, Flowsheet, Streams, and Blocks (with B1 and B2 expanded). The main workspace displays a "Reflux Ratio Profile" table:

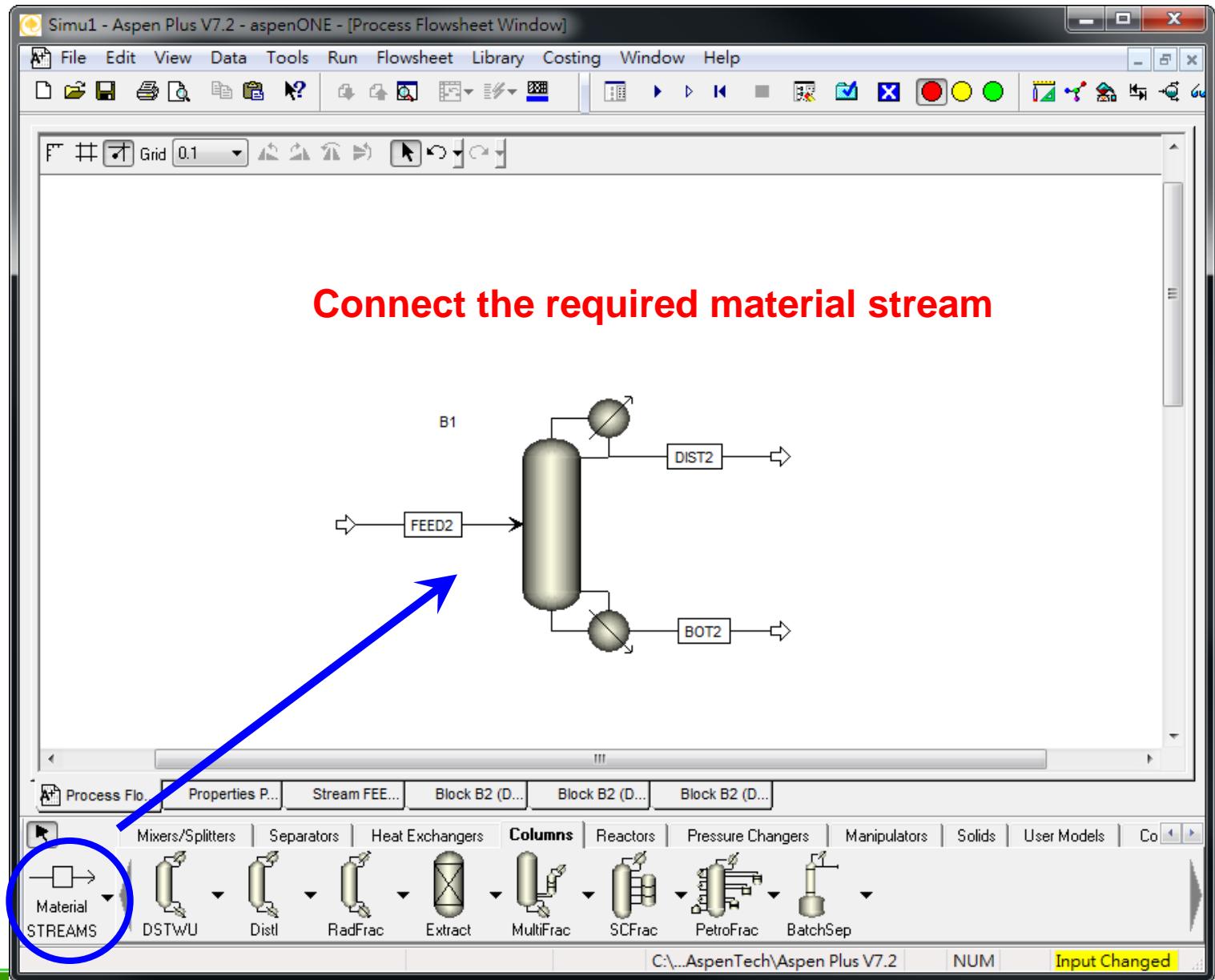
Theoretical stages	Reflux ratio
15	1.38489206
14	1.40081205
13	1.42216252
12	1.45300591
11	1.5040784
10	1.62109828
9	1.93292561
8	2.27429606
7	2.79611256
6	5.44420054

A red box highlights the last two rows of the table. A callout box on the right states: "For RR=3, at least 7 theoretical stages are required." The bottom navigation bar includes tabs for Process Flow, Properties P..., Stream FEE..., Block B2 (D..., and Block B2 (D...). The toolbar below the tabs includes icons for Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

3. More rigorous method in Aspen Plus (RADFRAC)



3. More rigorous method in Aspen Plus (RADFRAC)



3. More rigorous method in Aspen Plus (RADFRAC) (Feed Specification)

Simu1 - Aspen Plus V7.2 - aspenONE - [Stream FEED2 (MATERIAL) - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

FEED2 MET Specifications Flash Options PSD Component Attr. EO Options Costing

Substream name: MIXED Ref Temperature

State variables:

- Pressure: 100 kPa
- Vapor fraction: 0
- Total flow: Mole 100 kmol/hr
- Solvent:

Composition:

Component	Value
BEN	0.4
TOL	0.6

Total: 1

Same as Case 2

Input Changed. Unreconciled.

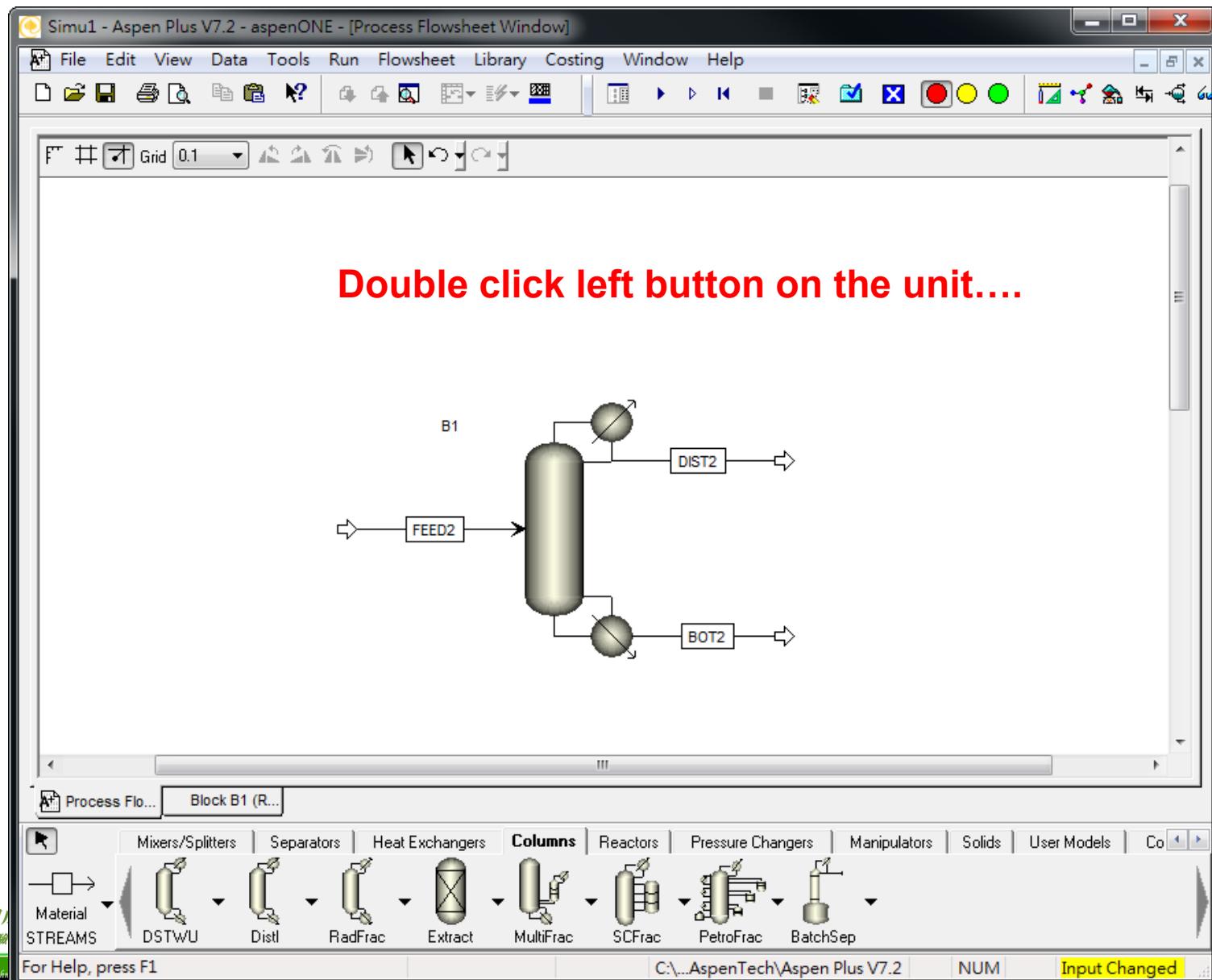
Process Flow Properties Stream FEE... Block B2 (D...) Block B2 (D...) Block B2 (D...) Stream FEED...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Column Specification)



3. More rigorous method in Aspen Plus (RADFRAC) (Column Specification)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar shows a tree view of the project structure under "B1": Streams, Blocks, and a detailed list of sub-blocks including Setup, Rate-based Distillation S., Design Specs, Vary, Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, Pack Rating, Properties, Estimates, and Convergence. A green circle highlights the "Configuration" tab in the top right corner of the main workspace. A red box highlights the "Number of stages" field set to 7 and the "Operating specifications" section where "Distillate rate" is set to 37.5 kmol/hr and "Reflux ratio" is set to 3. The bottom navigation bar includes tabs for Process Flow, Block B1 (Ra...), and various process equipment icons like Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The status bar at the bottom shows "Input Changed", "7 Stages 0 Pumparound(s)", "For Help, press F1", "C:\...AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

7 stages from previous calculation.

RR=3 from the problem, distillate rate = 37.5 (kmol/h) from previous calculation

3. More rigorous method in Aspen Plus (RADFRAC) (Column Specification)

The screenshot shows the Aspen Plus V7.2 software interface with the following details:

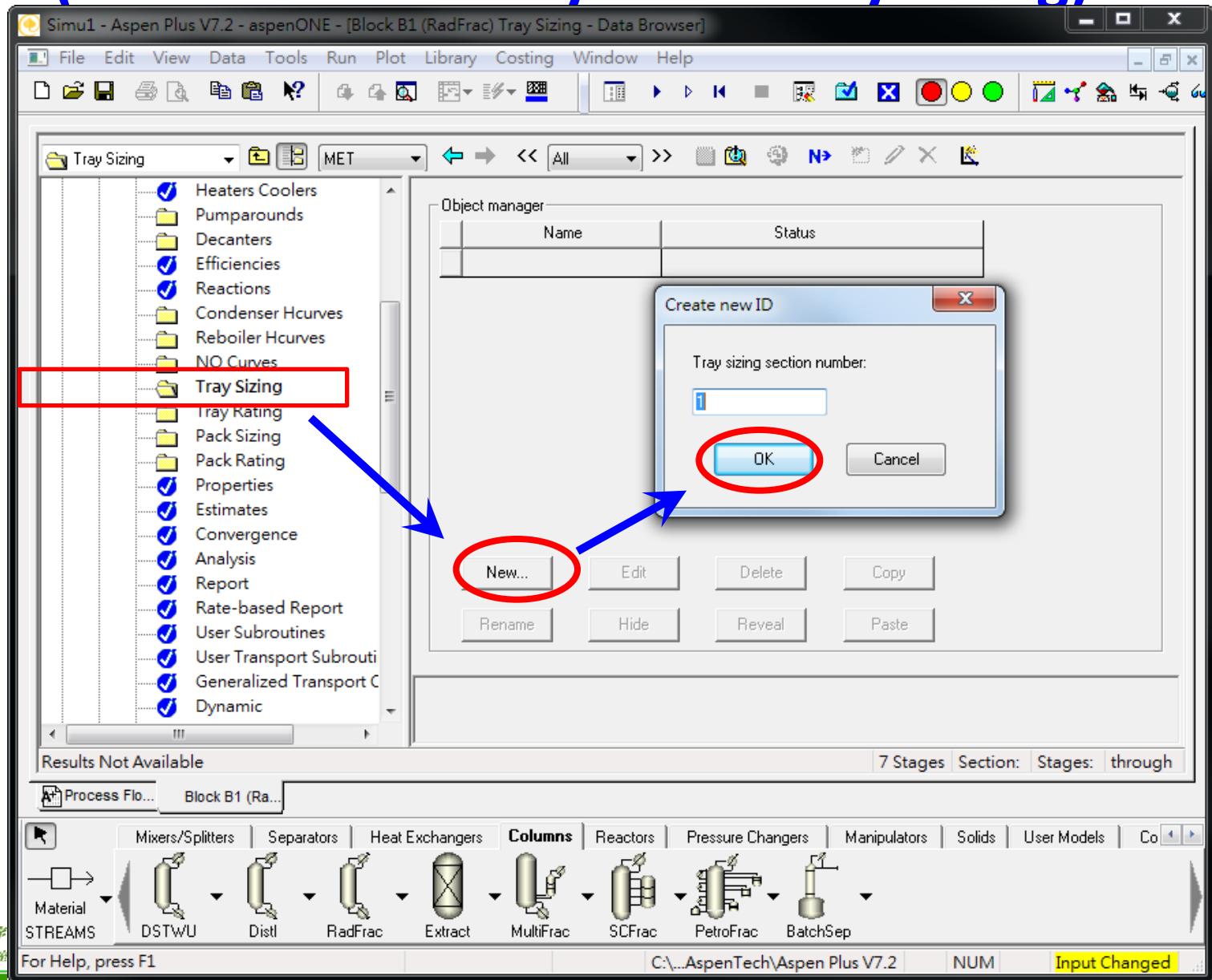
- Title Bar:** Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) - Data Browser]
- Menu Bar:** File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, Help
- Toolbars:** Standard toolbar with icons for file operations, zoom, and selection.
- Left Panel (Tree View):** Shows the project structure under B1, including Streams, Blocks, and various setup and design options like Setup, Rate-based Distillation, Design Specs, Vary, Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, Pack Rating, Properties, Estimates, and Convergence. A green circle highlights the "Streams" tab in the top navigation bar.
- Streams Tab Content:**
 - Feed streams:** A table with columns Name, Stage, and Convention. A red box highlights the "Stage" column for the FEED2 row, which is set to 4. The "Convention" column is set to On-Stage.
 - Product streams:** A table with columns Name, Stage, Phase, Basis, Flow, Units, and Flow ratio. It lists DIST2 (Stage 1, Liquid, Mole, kmol/hr) and BOT2 (Stage 7, Liquid, Mole, kmol/hr).
 - Text:** "Specify the feed stage."
 - Text:** "Feed stage number."
- Bottom Status Bar:** Input Changed, 7 Stages, 0 Pumparound(s)
- Bottom Toolbar:** Process Flow, Block B1 (Ra...), and various process equipment icons: Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.
- Bottom Navigation:** For Help, press F1, C:\...\AspenTech\Aspen Plus V7.2, NUM, Input Changed.

3. More rigorous method in Aspen Plus (RADFRAC) (Column Specification)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. On the left, a tree view shows the project structure with "B1" selected, containing "Streams", "Blocks", "Setup", "Rate-based Distillation S...", "Design Specs", "Vary", "Heaters Coolers", "Pumparounds", "Decanters", "Efficiencies", "Reactions", "Condenser Hcurves", "Reboiler Hcurves", "NQ Curves", "Tray Sizing", "Tray Rating", "Pack Sizing", "Pack Rating", "Properties", "Estimates", and "Convergence". A message "Input Changed" is displayed at the bottom left. The main panel shows "Configuration", "Streams", "Pressure" (highlighted with a green circle), "Condenser", "Thermosiphon Config.", "Reboiler", and "3-Phase" tabs. Under "Pressure", it says "Top stage / Condenser pressure" and "Stage 1 / Condenser pressure: 100 kPa". Below that are sections for "Stage 2 pressure (optional)" and "Pressure drop for rest of column (optional)". At the bottom, it says "7 Stages | 0 Pumparound(s)". The bottom navigation bar includes "Process Flow..." and "Block B1 (Ra...)" tabs, and categories like Mixers/Splitters, Separators, Heat Exchangers, Columns (highlighted with a blue box), Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The bottom status bar shows "For Help, press F1", "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

Specify the pressure at the top of column

3. More rigorous method in Aspen Plus (RADFRAC) (Calculation of tray size—Tray Sizing)

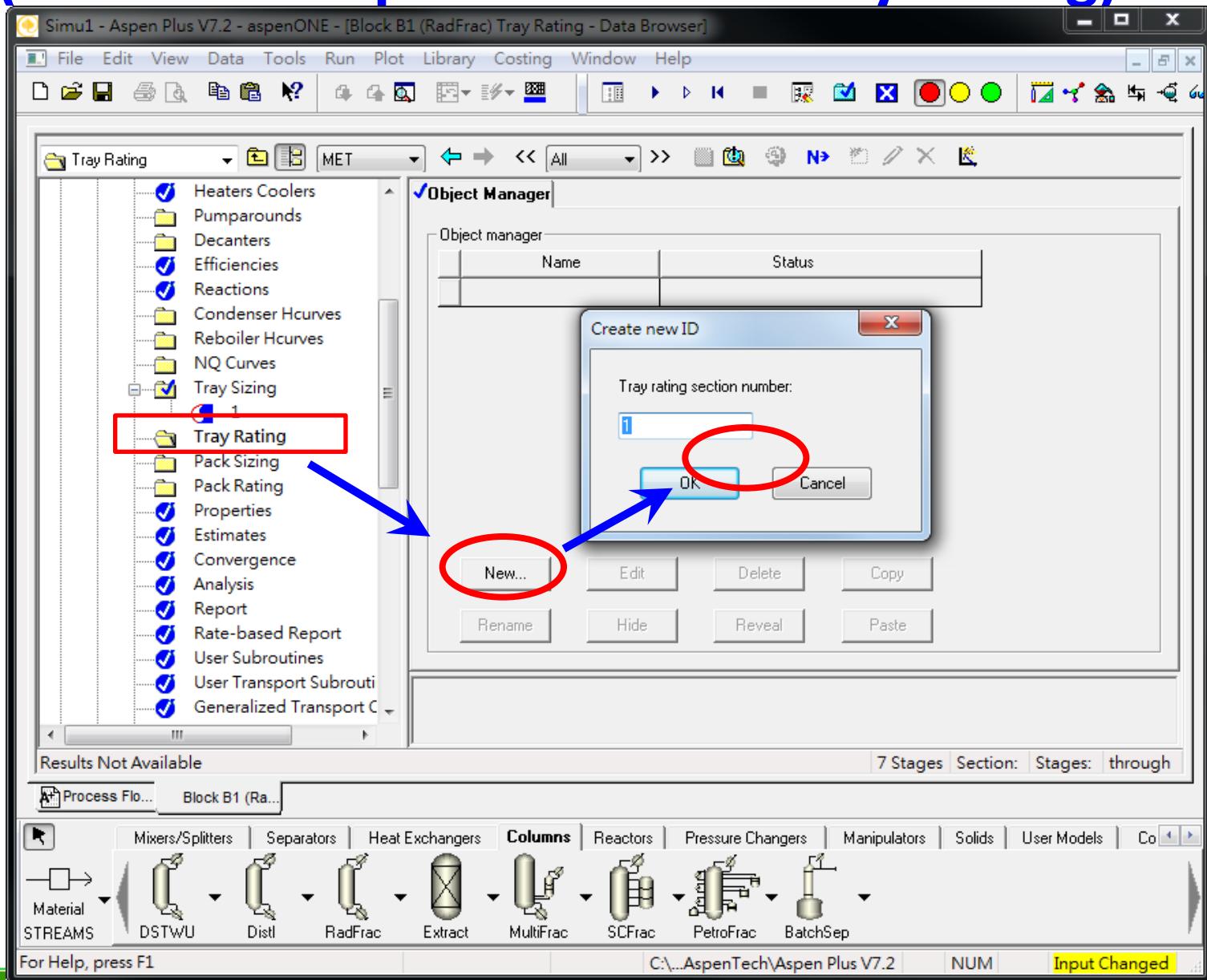


3. More rigorous method in Aspen Plus (RADFRAC) (Calculation of tray size—Tray Sizing)

*Calculation from 2th tray from the top to 2th tray from the bottom. (WHY???)

*Select a tray type.

3. More rigorous method in Aspen Plus (RADFRAC) (Pressure drop calculation– Tray Rating)

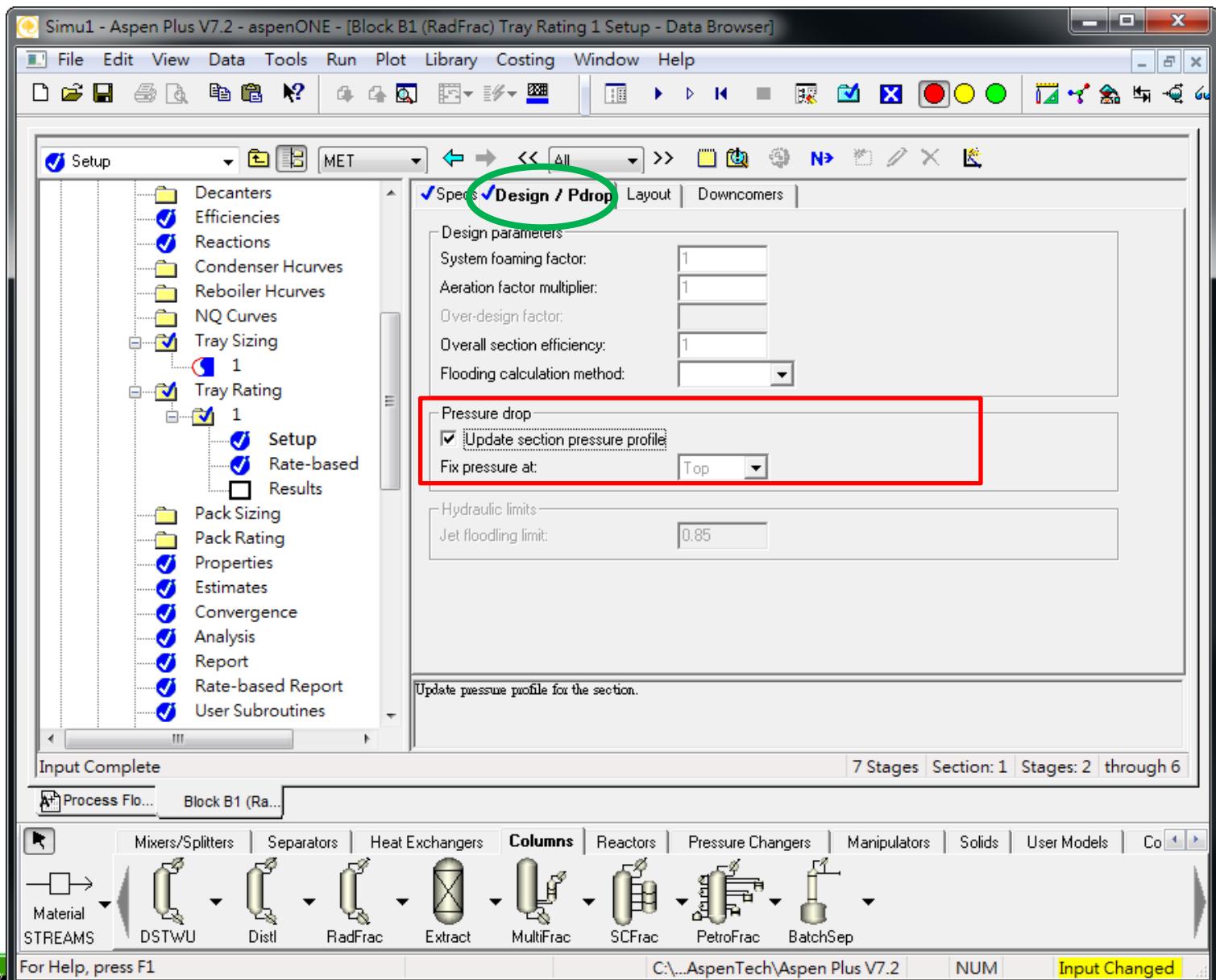


3. More rigorous method in Aspen Plus (RADFRAC) (Pressure drop calculation– Tray Rating)

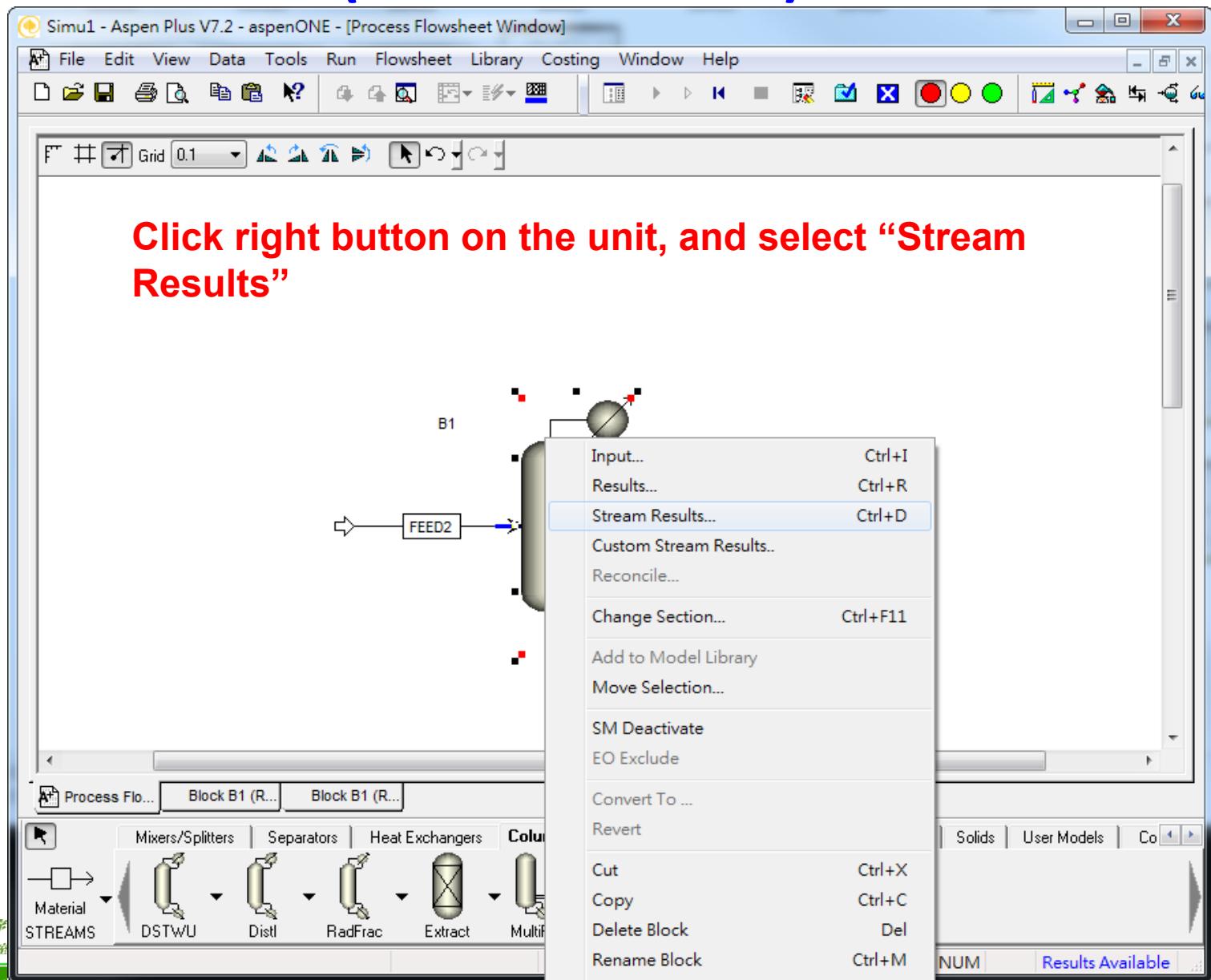
The screenshot shows the Aspen Plus V7.2 software interface. The main window title is "Simul1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Tray Rating 1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar has various icons for file operations. The left sidebar tree view shows categories like Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, and several sub-folders under Tray Sizing and Tray Rating, including Setup, Rate-based, Results, Pack Sizing, Pack Rating, Properties, Estimates, Convergence, Analysis, and Report. The central workspace is titled "Specs" and contains tabs for Design / Pdrop, Layout, and Downcomers. Under the "Trayed section" tab, there are fields for Starting stage (2), Ending stage (6), Tray type (Bubble Cap), and Number of passes (1). A red box highlights these four fields. Below them, under "Tray geometry", is a field for Diameter (1 meter) which is circled in red, and a field for Deck thickness (10 GAUGE). Under "Weir heights", there are four panels (A, B, C, D) each with a dropdown menu set to "meter". At the bottom of the workspace, it says "Input Complete" and "7 Stages Section: 1 Stages: 2 through 6". The bottom navigation bar includes Process Flow, Block B1 (Ra...), Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, Co, Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep. The status bar at the bottom shows "For Help, press F1", "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

*Calculation from 2th tray from the top to
2th tray from the bottom. (WHY???)
*Initial guess of the tray size

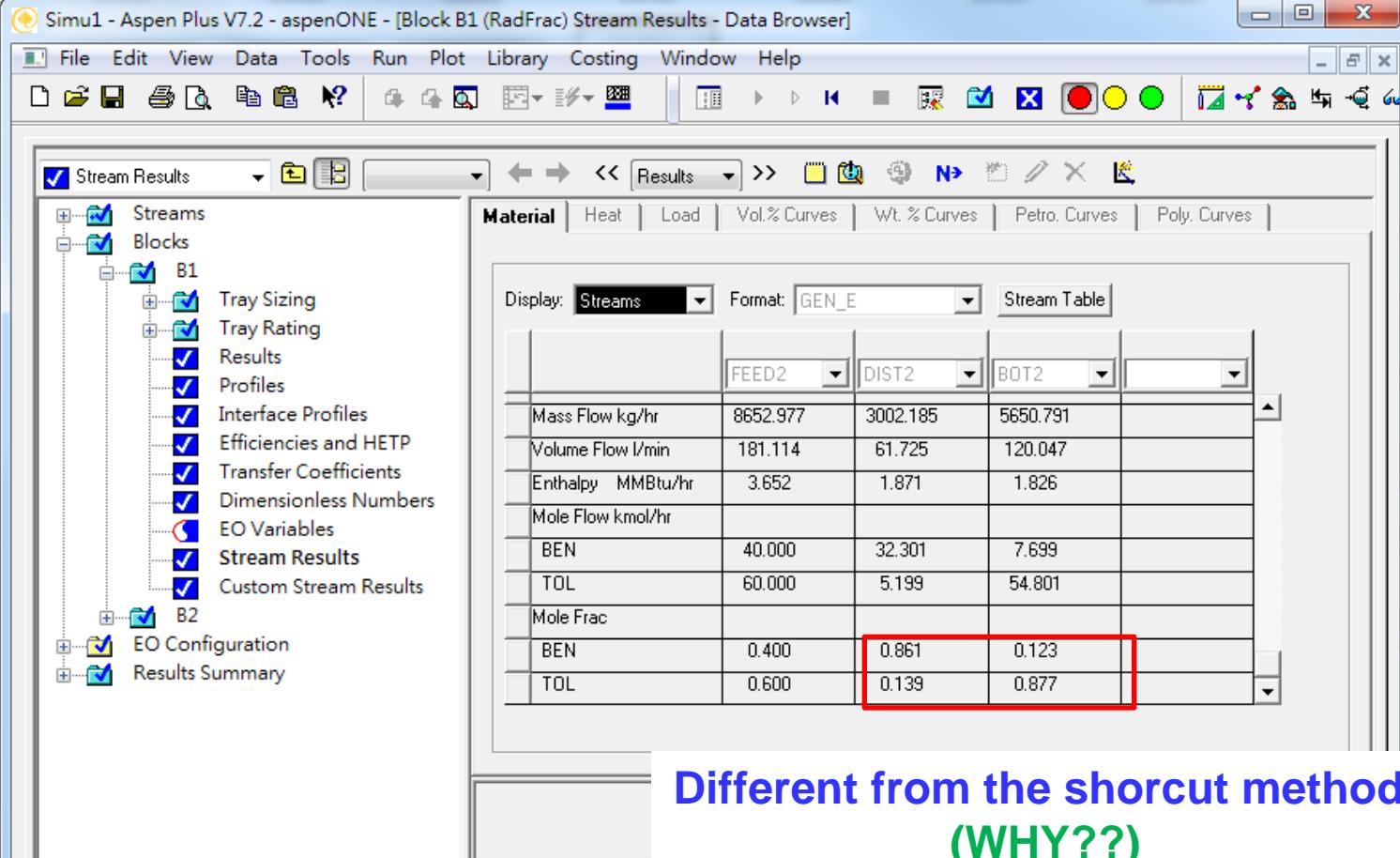
3. More rigorous method in Aspen Plus (RADFRAC) (Pressure drop calculation– Tray Rating)



3. More rigorous method in Aspen Plus (RADFRAC) (Stream Results)



3. More rigorous method in Aspen Plus (RADFRAC) (Stream Results)



The screenshot shows the Aspen Plus V7.2 interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Stream Results - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar shows a tree view of results: Stream Results, Streams, Blocks, B1 (Tray Sizing, Tray Rating, Results, Profiles, Interface Profiles, Efficiencies and HETP, Transfer Coefficients, Dimensionless Numbers, EO Variables, Stream Results, Custom Stream Results), B2, EO Configuration, and Results Summary. The main area has tabs for Material, Heat, Load, Vol.% Curves, Wt. % Curves, Petro. Curves, and Poly. Curves. The Stream Table tab is selected, displaying data for streams FEED2, DIST2, and BOT2. The table includes columns for Mass Flow kg/hr, Volume Flow l/min, Enthalpy MMBtu/hr, and Mole Flow kmol/hr. The Stream Table section also shows Mole Frac for BEN and TOL across the three streams. A red box highlights the mole fraction data for stream DIST2: BEN (0.861) and TOL (0.139).

Different from the shortcut method.
(WHY??)

Results Available

Process Flow Block B1 (R...) Block B1 (R...) Block B1 (Ra...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

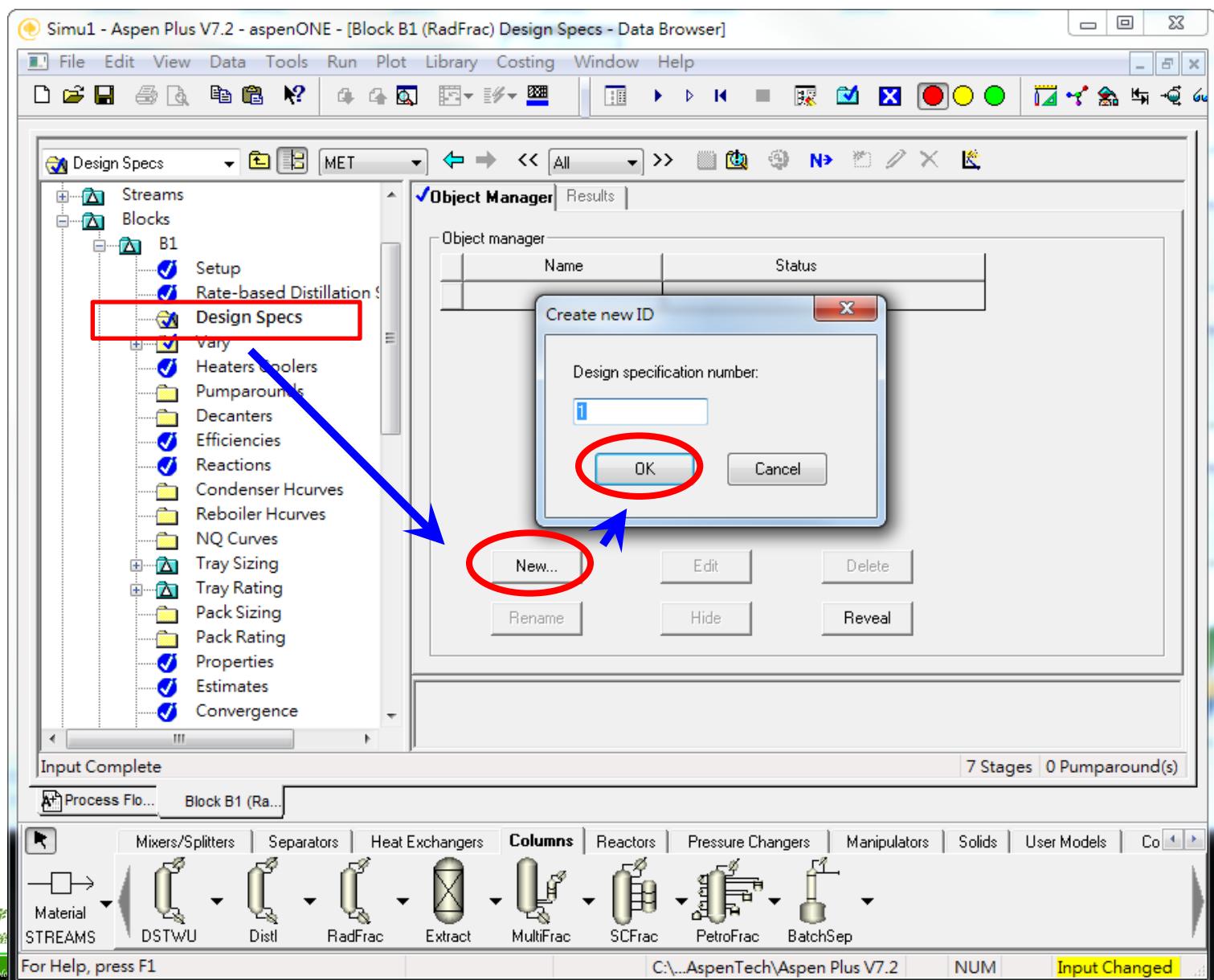
For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Results Available

Introduction to Aspen Plus

Part 7: Running simulation (Additional)

Design, spec, and vary in RADFRAC

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)



3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, Help. The toolbar has various icons for file operations and simulation. The left sidebar shows a tree view of the process: Streams, Blocks, B1 (Setup, Rate-based Distillation, Design Specs, Vary, Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, Pack Rating, Properties, Estimates). The main area is titled "Specifications" with tabs for Components, Feed/Product Streams, Options, and Results. Under "Design specification", the "Type" dropdown is set to "Mole purity", and the "Target" dropdown is empty. A tooltip below the target field says "Mole fraction of a group of components in a product, internal, or decanter stream." At the bottom, it says "Required Input Incomplete" and "7 Stages 0 Pumparound(s)". The bottom navigation bar includes Process Flow, Block B1 (Ra...), Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, Co..., Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, BatchSep. A status bar at the bottom says "For Help, press F1" and "C:\...\AspenTech\Aspen Plus V7.2".

**What do we want??
--- 90% Benzene at top.**

Select “Mole Purity”...

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation tasks.

The left sidebar displays a tree structure of process blocks and design specifications. Under "Blocks", "B1" is selected, showing "Setup", "Rate-based Distillation S", "Design Specs", "Vary", "Heaters Coolers", "Pumparounds", "Decanters", "Efficiencies", "Reactions", "Condenser Hcurves", "Reboiler Hcurves", "NQ Curves", "Tray Sizing", "Tray Rating", "Pack Sizing", "Pack Rating", "Properties", and "Estimates".

The main area is titled "Specifications" and includes sections for "Design specification" (Type: Mole purity), "Specification" (Target: 0.9), and "Stream type" (Product selected). A red box highlights the "Target" input field.

A callout box in the center-right of the screen contains the text:

What do we want??
--- 90% Benzene at top.

**Select “Mole Purity”...
And the target is 0.9.**

At the bottom, there are tabs for "Process Flow..." and "Block B1 (Ra...)".

The toolbar at the bottom includes icons for Material STREAMS, Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. Below the toolbar, specific unit icons are shown: DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

The status bar at the bottom shows "For Help, press F1", "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Required Input Incomplete".

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 1 - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Streams Blocks

B1

- Setup
- Rate-based Distillation S
- Design Specs
- 1
- Vary
- Heaters Coolers
- Pumparounds
- Decanters
- Efficiencies
- Reactions
- Condenser Hcurves
- Reboiler Hcurves
- NQ Curves
- Tray Sizing
- Tray Rating
- Pack Sizing
- Pack Rating
- Properties
- Estimates

Specifications Components Feed/Product Streams Options Results

Available components: TOL
Selected components: BEN

Base components: BEN TOL
Selected components:

C7H8 TOLUENE

Required Input Incomplete

7 Stages 0 Pumparound(s)

Process Flow Block B1 (Ra...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Required Input Incomplete

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar displays a tree structure with "Streams" and "Blocks" sections. Under "Blocks", "B1" is expanded, showing "Setup", "Rate-based Distillation S", "Design Specs", "Vary", "Heaters Coolers", "Pumparounds", "Decanters", "Efficiencies", "Reactions", "Condenser Hcurves", "Reboiler Hcurves", "NQ Curves", "Tray Sizing", "Tray Rating", "Pack Sizing", "Pack Rating", "Properties", and "Estimates". A green oval highlights the "Feed/Product Streams" tab in the top navigation bar, which is also labeled "Specifications", "Components", and "Feed/Product Streams". Below this, the "Available streams" list contains "BOT2", and the "Selected stream" list contains "DIST2". A callout text "Select the distillate stream" points to the "DIST2" entry. At the bottom, there are tabs for "Input Complete" and "Process Flow..." (active), and a status bar showing "7 Stages 0 Pumparound(s)". The bottom navigation bar includes icons for Material STREAMS, Mixers/Splitters, Separators, Heat Exchangers, Columns (selected), Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The "Columns" section of the toolbar shows icons for DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

Select the distillate stream

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Vary - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar shows a tree view of the process: Streams, Blocks, B1 (Setup, Rate-based Distillation S, Design Specs, Vary), and other categories like Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, Pack Rating, and Properties. A red box highlights the "Vary" node under B1. The main workspace displays the "Object Manager" dialog box, which has a sub-dialog titled "Create new ID" with the text "Adjusted variable number: 1" and an "OK" button circled in red. Below the main dialog are buttons for New..., Edit, Delete, Rename, Hide, and Reveal. To the right of the workspace, there is a callout box with the text "Add a Vary" and "(1 Design Spec ↔ 1 Vary)".

Add a Vary
(1 Design Spec ↔ 1 Vary)

Adjusted variable number:
1

OK Cancel

New... Edit Delete Rename Hide Reveal

Input Complete 7 Stages 0 Pumparound(s)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Vary 1 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation. The left sidebar lists "Streams", "Blocks", and specific items like "Setup", "Rate-based Distillation S", "Design Specs", "Vary", "Heaters Coolers", "Pumparounds", "Decanters", "Efficiencies", "Reactions", "Condenser Hcurves", "Reboiler Hcurves", "NQ Curves", "Tray Sizing", "Tray Rating", "Pack Sizing", "Pack Rating", and "Properties". The main area has tabs for "Specifications", "Components", and "Results". The "Specifications" tab is active, showing the "Adjusted variable" section with "Type: Reflux ratio" selected from a dropdown menu. Other options in the dropdown include Boilup ratio, Condenser duty, Reboiler duty, Free water reflux ratio, Liquid sidestream rate, Vapor sidestream rate, External duty, Feed rate, Inlet heat stream duty, Murphree efficiency, Thermosiphon temp, Thermosiphon temp change, Thermosiphon vapor fraction, Thermosiphon flow, 1st liquid return fraction, 2nd liquid return fraction, Pumparound flow, Pumparound temp, and Pumparound temp change. Below the dropdown is a note: "Reflux ratio (liquid reflux/distillate) which excludes free water for all cases except when Valid Phases=Vapor-Liquid-FreeWaterAnyStage (Setup Configuration sheet)." At the bottom, there are buttons for "Input Complete", "Process Flow...", "Block B1 (Ra...", and "7 Stages | 0 Pumparound(s)". The bottom navigation bar includes icons for Material Streams, Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and more. The status bar at the bottom shows "For Help, press F1", "C:\...AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

Varying Reflux ratio to reach the design target.

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. On the left, the navigation tree displays the project structure under 'B1'. The 'Design Specs' section is selected, showing a 'Reflux ratio' specification with its type set to 'Reflux ratio'. The 'Upper and lower bounds' field is highlighted with a red box, containing values '0' and '10' respectively. Below this, an optional 'Maximum step size' field is present. A callout box with the text 'Specify the varying range.
(Should contain the initial value)' points to the 'Upper and lower bounds' field.

Specify the varying range.
(Should contain the initial value)

Reflux ratio

Phases=Vapor-Liquid-FreeWaterAnyStage (Setup Configuration sheet).

Streams
Blocks
B1
Setup
Rate-based Distillation
Design Specs
1
Vary
1
Heaters Coolers
Pumparounds
Decanters
Efficiencies
Reactions
Condenser Hcurves
Reboiler Hcurves
NQ Curves
Tray Sizing
Tray Rating
Pack Sizing
Pack Rating
Properties

Adjusted variable
Type: Reflux ratio
Upper and lower bounds
Lower bound: 0
Upper bound: 10
Optional
Maximum step size:

Input Complete

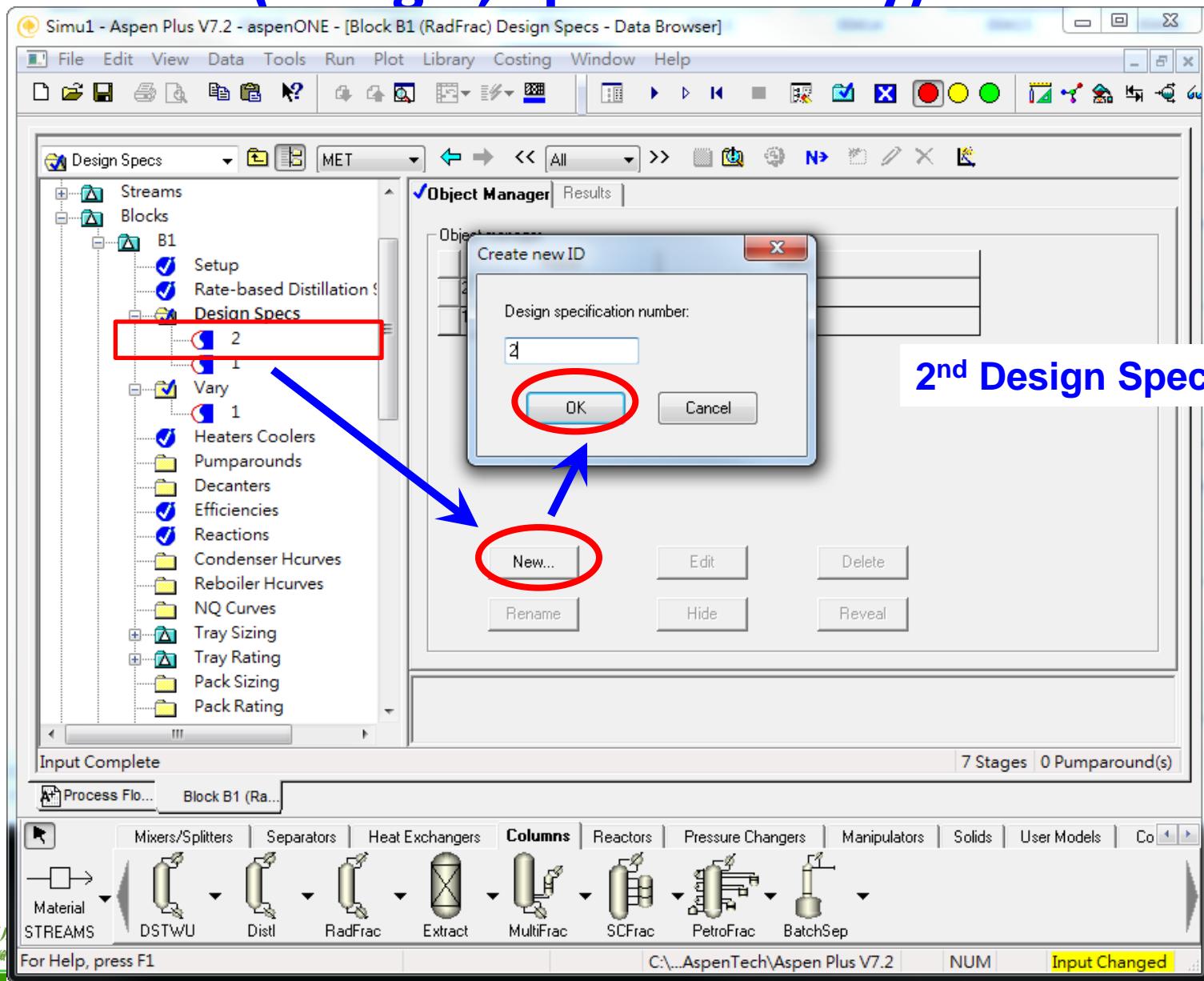
Process Flow Block B1 (Ra...
Material STREAMS
DSTWU
Distl
RadFrac
Extract
MultiFrac
SCFrac
PetroFrac
BatchSep

7 Stages 0 Pumparound(s)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)



3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 2 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar has various icons for file operations and simulation. The left sidebar lists "Streams" and "Blocks". Under "Blocks", "B1" is expanded to show "Setup", "Rate-based Distillation", "Design Specs", "Vary", and other sub-blocks like Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, and Pack Rating. The "Design Specs" section is selected. It contains fields for "Type" (set to "Mole purity"), "Specification" (set to "Target"), and "Stream type" (set to "Product"). A dropdown menu under "Type" lists numerous options, with "Mole purity" highlighted. A tooltip below the dropdown explains: "Mole fraction of a group of components in a product, internal, or decanter stream." At the bottom, tabs for "Input Complete" and "Process Flow..." are visible, along with a status bar showing "7 Stages 0 Pumparound(s)". The bottom navigation bar includes icons for Material STREAMS, Mixers/Splitters, Separators, Heat Exchangers, Columns (selected), Reactors, Pressure Changers, Manipulators, Solids, User Models, and a "Co" button. Below the navigation bar, there are buttons for DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

What do we want??
--- 10% Benzene at bot.

Select “Mole Purity”...

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 2 - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Streams Blocks

B1

- Setup
- Rate-based Distillation S
- Design Specs
- 2
- 1
- Vary
- 2
- Heaters Coolers
- Pumparounds
- Decanters
- Efficiencies
- Reactions
- Condenser Hcurves
- Reboiler Hcurves
- NQ Curves
- Tray Sizing
- Tray Rating
- Pack Sizing
- Pack Rating

Specifications Components Feed/Product Streams Options Results

Type: Mole purity

Specification Target: 0.1

Stream type: Product

What do we want??
--- 10% Benzene at bot.

Select “Mole Purity”...
And the target is 0.1.

Input Complete 7 Stages 0 Pumparound(s)

Process Flow Block B1 (Ra... Columns Reactors Pressure Changers Manipulators Solids User Models Co

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 2 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar has various icons for file operations and simulation. On the left, the navigation tree shows "Streams", "Blocks", "B1" (selected), "Setup", "Rate-based Distillation", "Design Specs" (selected), "Vary", and other process components like Heaters Coolers, Pumparounds, Decanters, Efficiencies, Reactions, Condenser Hcurves, Reboiler Hcurves, NQ Curves, Tray Sizing, Tray Rating, Pack Sizing, and Pack Rating. The main workspace is titled "Components" and shows two sections: "Available components" containing "TOL" and "Selected components" containing "BEN". Below this, "Base components" show "BEN" and "TOL". A status bar at the bottom indicates "Input Complete", "7 Stages | 0 Pumparound(s)", and toolbars for Process Flow and Block B1 (RadFrac). A legend at the bottom shows symbols for Material STREAMS, Mixers/Splitters, Separators, Heat Exchangers, Columns (highlighted), Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The bottom status bar also includes "For Help, press F1", the path "C:\...AspenTech\Aspen Plus V7.2", and "NUM Input Changed".

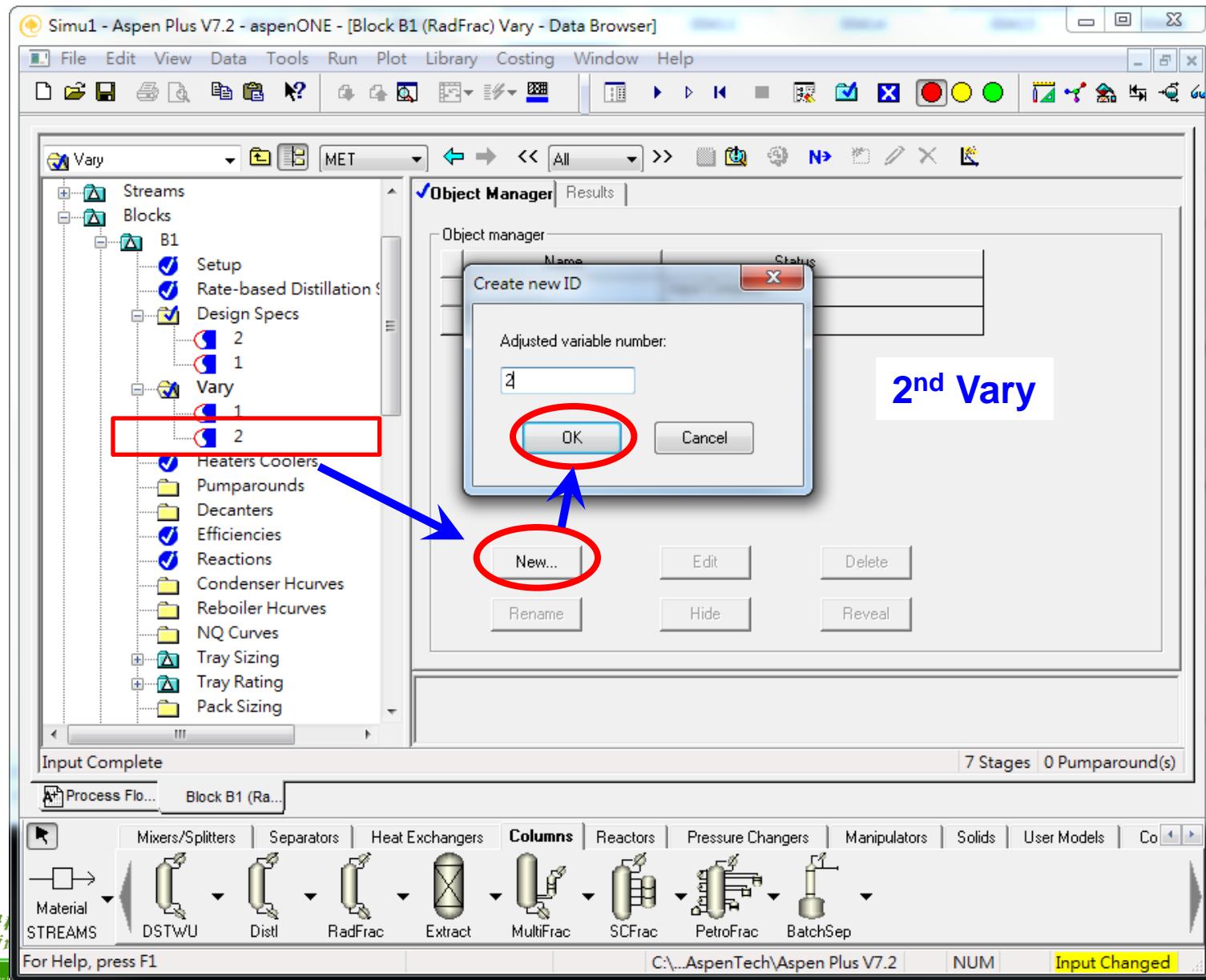
Select the Benzene

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

The screenshot shows the Aspen Plus V7.2 software interface with the title bar "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Design Specs 2 - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar has various icons for file operations like Open, Save, Print, and zoom. The left sidebar shows a tree structure with "Streams" and "Blocks". Under "Blocks", "B1" is expanded, showing "Setup", "Rate-based Distillation S", "Design Specs" (which is checked), "Vary", "Heaters Coolers", "Pumparounds", "Decanters", "Efficiencies", "Reactions", "Condenser Hcurves", "Reboiler Hcurves", "NQ Curves", "Tray Sizing", "Tray Rating", "Pack Sizing", and "Pack Rating". The "Design Specs" section has two sub-options: "2" and "1". The main workspace is titled "Design Specs" and includes tabs for "Specifications", "Components", and "Feed/Product Streams" (which is circled in green). Below these tabs are sections for "Product streams" (with "Available streams" list containing "DIST2" and "Selected stream" list containing "BOT2") and "Feed/Product streams as base streams". A note at the bottom says "Product streams to include in the specification." At the bottom of the screen, there's a toolbar with icons for Process Flow, Block B1 (Ra...), Mixers/Splitters, Separators, Heat Exchangers, Columns (highlighted in blue), Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The status bar at the bottom shows "Input Complete", "7 Stages 0 Pumparound(s)", "For Help, press F1", "C:\...\AspenTech\Aspen Plus V7.2", "NUM", and "Input Changed".

Select the bottom stream

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)



3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Vary 2 - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Streams Blocks

B1

- Setup
- Rate-based Distillation S
- Design Specs
- 2
- 1
- Vary
- 1
- 2
- Heaters Coolers
- Pumparounds
- Decanters
- Efficiencies
- Reactions
- Condenser Hcurves
- Reboiler Hcurves
- NQ Curves
- Tray Sizing
- Tray Rating
- Pack Sizing

Adjusted variable

Type: Distillate rate

Upper and lower bounds

Lower bound: 35 kmol/hr

Upper bound: 55 kmol/hr

Optional

Maximum step size:

Varying distillate rate to reach the design target.

Specify the varying range.
(Should contain the initial value)

Upper bound for the manipulated variable. Units for the upper bound are Type units from the block Units-Set.

Input Complete

Process Flow... Block B1 (Ra...

7 Stages 0 Pumparound(s)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS

DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Design , Spec and Vary)

Simu1 - Aspen Plus V7.2 - aspenONE - [Process Flowsheet Window]

File Edit View Data Tools Run Flowsheet Library Costing Window Help

Grid 0.1

B1
FEED2
DIST2
BOT2

RUN THE SIMULATION,
and click right button on
the unit, select “Stream
results”

Process Flo... Block B1 (R... Block B1 (R... Block B1 (R... Stream FEE... Block B1 (R... Block B1 (R...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Input Changed

3. More rigorous method in Aspen Plus (RADFRAC) (Stream Results)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Stream Results - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Streams Blocks B1 Design Specs Vary Tray Sizing Tray Rating Results Profiles Interface Profiles Efficiencies and HETP Transfer Coefficients Dimensionless Numbers EO Variables Stream Results Custom Stream Results B2 EO Configuration Results Summary

Material Heat Load Vol.% Curves Wt. % Curves Petro. Curves Poly. Curves

Display: Streams Format: GEN_E Stream Table

	FEED2	DIST2	BOT2	
Mass Flow kg/hr	8652.977	2981.862	5671.114	
Volume Flow l/min	181.524	61.218	120.912	
Enthalpy MMBtu/hr	3.682	1.915	1.808	
Mole Flow kmol/hr				
BEN	40.000	33.750	6.250	
TOL	60.000	3.750	56.250	
Mole Frac				
BEN	0.400	0.900	0.100	
TOL	0.600	0.100	0.900	

The required product quality

Results Available. Unreconciled. 7 Stages | 0 Pumparound(s)

Process Flow Block B1 (R...) Block B1 (R...) Block B1 (R...) Stream FEE... Block B1 (Ra...
Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co 1
Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep
For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Results Available

3. More rigorous method in Aspen Plus (RADFRAC) (Column Results--top)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Results - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Results

Convergence Analysis Report Rate-based Report User Subroutines User Transport Subroutine Generalized Transport C Dynamic Dynamic Equipment HT Block Options Results Profiles Interface Profiles Efficiencies and HETP Transfer Coefficients Dimensionless Numbers EO Variables EO Input Spec Groups Ports Stream Results Custom Stream Results

Summary Balance Split Fraction Reboiler Utilities Stage Utilities

View: Condenser / Top stage Basis: Mole

Condenser / Top stage performance

Temperature:	354.886566 K
Subcooled Temperature:	
Heat duty:	-556496.54 cal/sec
Subcooled duty:	
Distillate rate:	37.4999999 kmol/hr
Reflux rate:	230.289809 kmol/hr
Reflux ratio:	6.14106159

Calculated Reflux Ratio = 6.14
(from problem: 3)

Select view option.

Results Available. Unreconciled. 7 Stages 0 Pumparound(s)

Process Flow... Block B1 (R...) Block B1 (R...) Block B1 (R...) Stream FEE... Block B1 (R...) Block B1 (Ra...)

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co...

Material STREAMS DSTWU Dist RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...\AspenTech\Aspen Plus V7.2 NUM Results Available

3. More rigorous method in Aspen Plus (RADFRAC) (Column Results--bottom)

The required heat duty for separation is 2341.8 (KW)

Results Available. Unreconciled.

7 Stages | 0 Pumparound(s)

Process Flow | Block B1 (R...) | Block B1 (R...) | Block B1 (R...) | Stream FEE... | Block B1 (R...) | Block B1 (Ra...)

Mixers/Splitters | Separators | Heat Exchangers | **Columns** | Reactors | Pressure Changers | Manipulators | Solids | User Models | Co...

Material STREAMS

DSTWU | Distl | RadFrac | Extract | MultiFrac | SCFrac | PetroFrac | BatchSep

For Help, press F1 | C:\...\AspenTech\Aspen Plus V7.2 | NUM | Results Available

3. More rigorous method in Aspen Plus (RADFRAC) (Profile Inside the Column)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Profiles - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Profiles

TPFQ (circled in red)

View: Summary Basis: Mole

Profiles

Stage	Temperature	Pressure	Heat duty	Liquid from	Vapor from
	K	atm	cal/sec	kmol/hr	kmol/hr
1	354.886562	0.98692327	-556437.5	267.758641	0
2	357.532549	0.98692327	0	225.850699	267.758641
3	362.399742	1.00640034	0	221.67864	263.350699
4	368.205689	1.02571776	0	318.523818	259.178641
5	373.189296	1.04582401	0	316.762888	256.023818
6	378.194545	1.06573423	0	316.037914	254.262888
7	382.336307	1.085778	559269.877	62.4999997	253.537914

T : Temperature
P : Pressure
F : Liquid and vapor flow rate.
Q: Heat Duty

Process Flow Block B1 (R...) Block B1 (R...) Block B1

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co

Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

For Help, press F1 C:\...AspenTech\Aspen Plus V7.2 NUM Results Available

3. More rigorous method in Aspen Plus (RADFRAC) (Profile Inside the Column)

The screenshot shows the Aspen Plus V7.2 software interface. The title bar reads "Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Profiles - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, Help. The toolbar has various icons for file operations. The left sidebar has a tree view with checked items: Pack Sizing, Pack Rating, Properties, Estimates, Convergence, Analysis, Report, Rate-based Report, User Subroutines, User Transport Subroutine, Generalized Transport C, Dynamic, Dynamic Equipment HT, Block Options, Results, and Profiles (which is selected and highlighted with a red box). The main area has tabs: TPFQ, Compositions (circled in red), K-Values, Hydraulics, Reactions, Efficiencies, Properties, and Key Cc. The "View:" dropdown is set to "Vapor" and the "Basis:" dropdown is set to "Mole". The "Composition profiles" table shows the following data:

Stage	BEN	TOL
1	0.95822378	0.04177621
2	0.89999977	0.10000023
3	0.79691352	0.20308648
4	0.65144156	0.34855844
5	0.51116773	0.48883227
6	0.35041919	0.64958081
7	0.20583252	0.79416748

You can select the vapor or liquid composition profile. (also in mole or mass basis)

At the bottom, there are tabs for Process Flow, Block B1 (R...), Stream FEE..., and other process components like Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, User Models, and Co. The Columns tab is currently selected. Below the tabs are icons for Material STREAMS, DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, and BatchSep.

3. More rigorous method in Aspen Plus (RADFRAC) (Plotting Temp. Profile)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Profiles - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

X-Axis Variable Ctrl+Alt+X
Y-Axis Variable Ctrl+Alt+Y
Parametric Variable Ctrl+Alt+Z
Display Plot Ctrl+Alt+P
Add New Curve...
Plot Wizard... Ctrl+Alt+W

Basis: Mole

	K	atm	cal/sec	kmol/hr	kmol/hr
1	354.886562	0.98692327	-556437.5	267.758641	0
2	357.532549	0.98692327	0	225.850699	267.758641
3	362.399742	1.00640034	0	221.67864	263.350699
4	368.205689	1.02571776	0	318.523818	259.178641
5	373.189296	1.04582401	0	316.762888	256.023818
6	378.194545	1.06573423	0	316.037914	254.262888
7	382.336307	1.085778	559269.877	62.4999997	253.537914

Select the column “Stage”
Click “Plot”
Select “X-axis variable”

Process Flo... Block B1 (R... Block B1 (R... Block B1 (R... Stream FEE... Block B1 (R... Block B1 (R... Block B1 (R...
Mixer/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co...
Material STREAMS DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

Selects the x axis variable for plotting C:\...AspenTech\Aspen Plus V7.2 NUM Results Available

3. More rigorous method in Aspen Plus (RADFRAC) (Plotting Temp. Profile)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Profiles - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Plot Type...
X-Axis Variable Ctrl+Alt+X
Y-Axis Variable Ctrl+Alt+Y
Parametric Variable Ctrl+Alt+Z
Display Plot Ctrl+Alt+P
Add New Curve...
Plot Wizard... Ctrl+Alt+W

Basis: Mole

	K	atm	cal/sec	kmol/hr	kmol/hr
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6	378.194545	1.06573423	0	316.037914	254.262888
7	382.336307	1.085778	559269.877	62.4999997	253.537914

Select the column “Temp.”

Click “Plot”

Select “Y-axis variable”

Results Available. Unreconciled. 7 Stages 0 Pumparound(s)

Process Flow Block B1 (R...) Block B1 (R...) Block B1 (R...) Stream FEE... Block B1 (R...) Block B1 (R...) Block B1 (Ra...
Mixer/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co...
Material STREAMS DSTwU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

Selects the y axis variable for plotting C:\...AspenTech\Aspen Plus V7.2 NUM Results Available

Green Chemical Process Technology

3. More rigorous method in Aspen Plus (RADFRAC) (Plotting Temp. Profile)

Simu1 - Aspen Plus V7.2 - aspenONE - [Block B1 (RadFrac) Profiles - Data Browser]

File Edit View Data Tools Run Plot Library Costing Window Help

Profiles

- Tray Rating
- Pack Sizing
- Pack Rating
- Properties
- Estimates
- Convergence
- Analysis
- Report
- Rate-based Report
- User Subroutines
- User Transport Subroutine
- Generalized Transport C
- Dynamic
- Dynamic Equipment HT
- Block Options
- Results
- Profiles
- Interface Profiles
- Efficiencies and HETP
- Transfer Coefficients
- Dimensionless Numbers
- EO Variables

Plot Type... X-Axis Variable Ctrl+Alt+X
Y-Axis Variable Ctrl+Alt+Y
Parametric Variable Ctrl+Alt+Z
Display Plot Ctrl+Alt+P
Add New Curve...
Plot Wizard... Ctrl+Alt+W

Basis: Mole

	K	atm	cal/sec	kmol/hr	kmol/hr
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7	382.336307	1.085778	559269.877	62.4999997	253.537914

Results Available. Unreconciled.

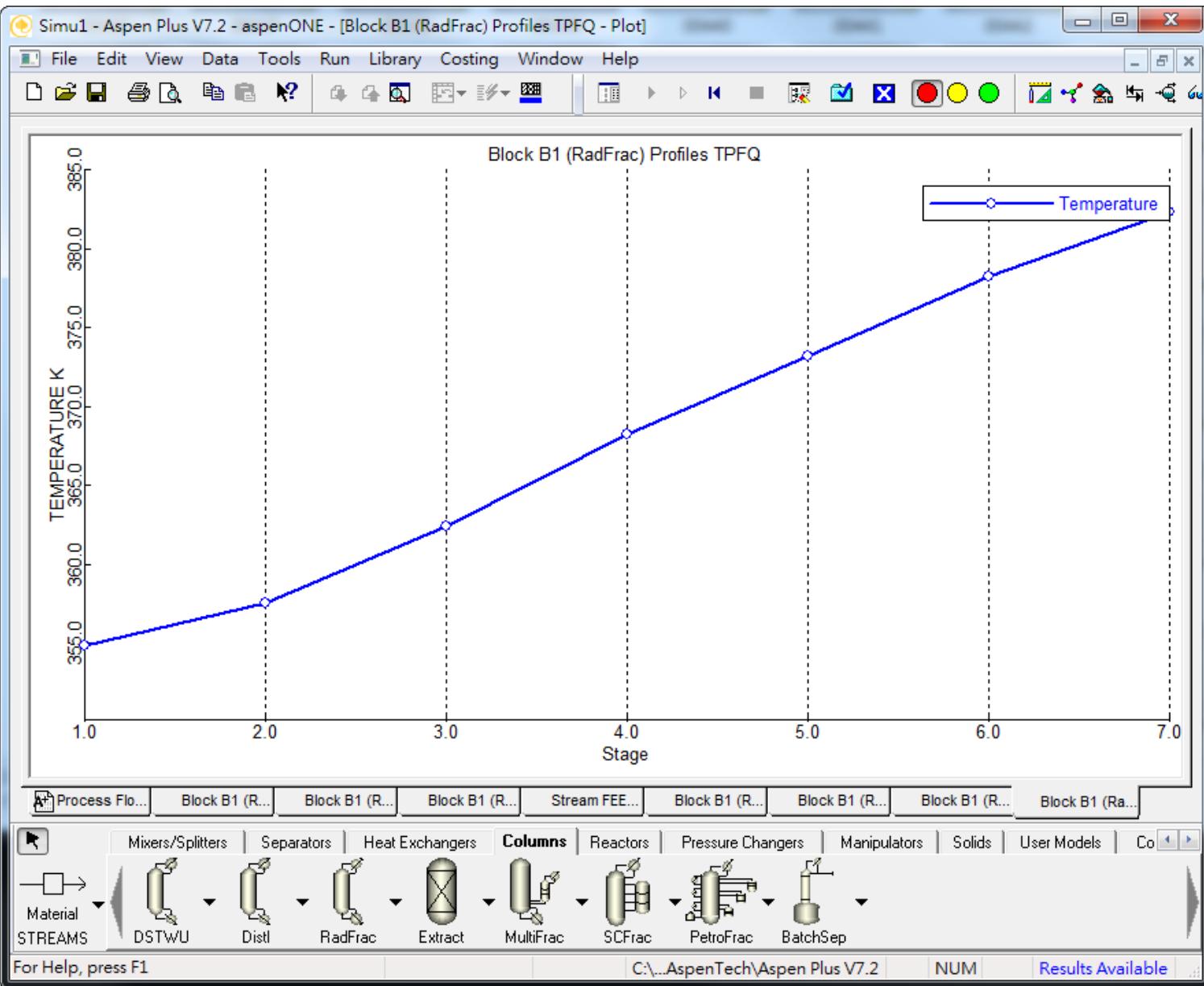
7 Stages 0 Pumparound(s)

Process Flow Block B1 (R...) Block B1 (R...) Stream FEE... Block B1 (R...) Block B1 (R...) Block B1 (R...) Block B1 (R...) Block B1 (Ra...
Material STREAMS Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Co...
DSTWU Distl RadFrac Extract MultiFrac SCFrac PetroFrac BatchSep

Displays a plot based on the current default setti C:\...\AspenTech\Aspen Plus V7.2 NUM Results Available

Then, select “Display Plot”

3. More rigorous method in Aspen Plus (RADFRAC) (Plotting Temp. Profile)



Exercise

Example:

Typically, 90 mol% product purity is not enough for a product to sale. In the same problem, assume the number of stages increase to 10. Try the following exercises:

- (1) Is it possible to separate the feed to 95 mol% of benzene in the distillate, and less than 5% of benzene in the bottom product? If yes, what is the RR and Qreb?
- (2) As in (1), is it possible to separate the feed to 99 mol% of benzene in the distillate, and less than 1% of benzene in the bottom product? If yes, what is the RR and Qreb?
- (3) As in (2), if no, how many number of stages is required to reach this target?

(Hint: Use design, spec, and vary to do this problem)

Thanks for your attention!

PSE Laboratory
Department of Chemical Engineering
National Taiwan University
(綜合 room 402)