Introduction
to
Aspen Plus Basics
version 10.2

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Course Agenda – day 1

Introduction - General Simulation Concepts

The User Interface - Graphical Flowsheet Definition

Basic Input - Getting Around the Graphical User Interface

Unit Operation Models - Overview of Available Unit Operations

Separator – Two-phase & Three-phase Flash Calculation

DSTWU – Determination of N_{min} and R_{min}

DISTIL – Preliminary Separation Approximation

RadFrac - Multistage Separation Model

Course Agenda – day 1

Heat Exchangers - Heaters and Heat Exchangers

Pressure Changers - Pumps, Compressors, Pipes and Valves

Reactor Models - Overview of Available Reactor Types

Full-Scale Plant Modeling Workshop : *Additional*

- Simulate a Methanol Plant
- Simulate a PX Plant
- Simulate a CDU

Introduction

Objective:

Introduce general flowsheet simulation concepts and Aspen Plus features

Introduction

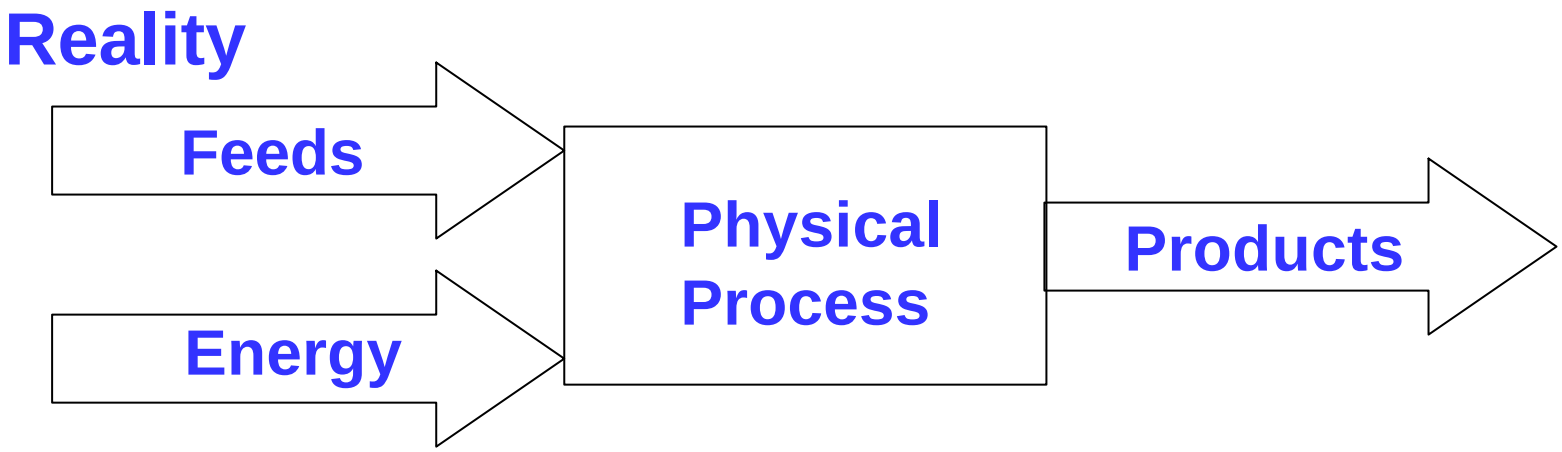
- What is flowsheet simulation?
  - Use of a computer program to quantitatively model the characteristic equations of a chemical process
- Uses underlying physical relationships
  - Mass balance
  - Equilibrium relationships
  - Summation of Compositions
  - Enthalpy Balance
  - Rate correlations (reaction and mass/heat transfer)
- Predicts
  - Stream flowrates, compositions and physical properties
  - Operating conditions
  - Equipment sizing

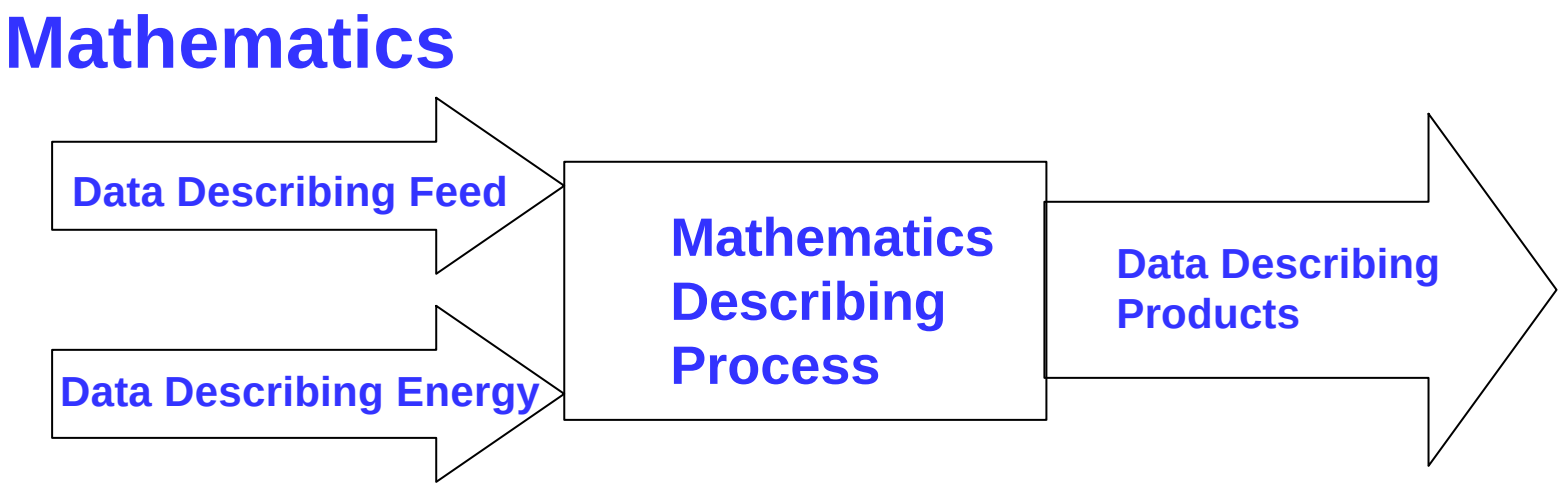
화학공정 모사기란 무엇인가?

- 화학공정 모사기(Chemical Process Simulator)는 화학공정을 **열역학**을 이용하여 수학적으로 모델화하여서 이를 Computer Hardware를 이용하여 실제 공장에서 일어나는 상황을 묘사하는 Software이다. - 1988

Henry Jo

Process Simulation





공정모사의 목적
(Purposes for Simulation?)

- 새로운 공장의 설계

  New Plant Design

- 기존 공장의 개조 (증설)

  Existing Plant Revamp (Expansion)

- 기존 공장의 운전조건 진단

  Existing Plant Operations

- 교육 훈련

  Engineer Training

Advantages of Simulation

- Reduces plant design time
  - Allows designer to quickly test various plant configurations
- Helps improve current process
  - Answers “what if” questions
  - Determines optimal process conditions within given constraints
  - Assists in locating the constraining parts of a process (debottlenecking)

공정 모사의 장점
Advantages of Simulation

- Faster Calculations - More solutions
- Accurate Results
- Standardization
  - Pure Components : 1,550개
  - Binary Database : 10,000 VLE & 3,000 LLE
  - Thermodynamic Methods over 60 Models
- Solution of Recycle Processes
- Less Costly than Pilot Plant Tests !!

공정 모사의 장점 (I)
Faster Calculations

- The equilibrium flash separator is the simplest equilibrium-stage process with which the designer must deal. Despite the fact that only one stage is involved, the calculation of the compositions and the relative amount of the vapor and liquid phases at any given pressure and temperature usually involves a tedious trial-and-error solution.

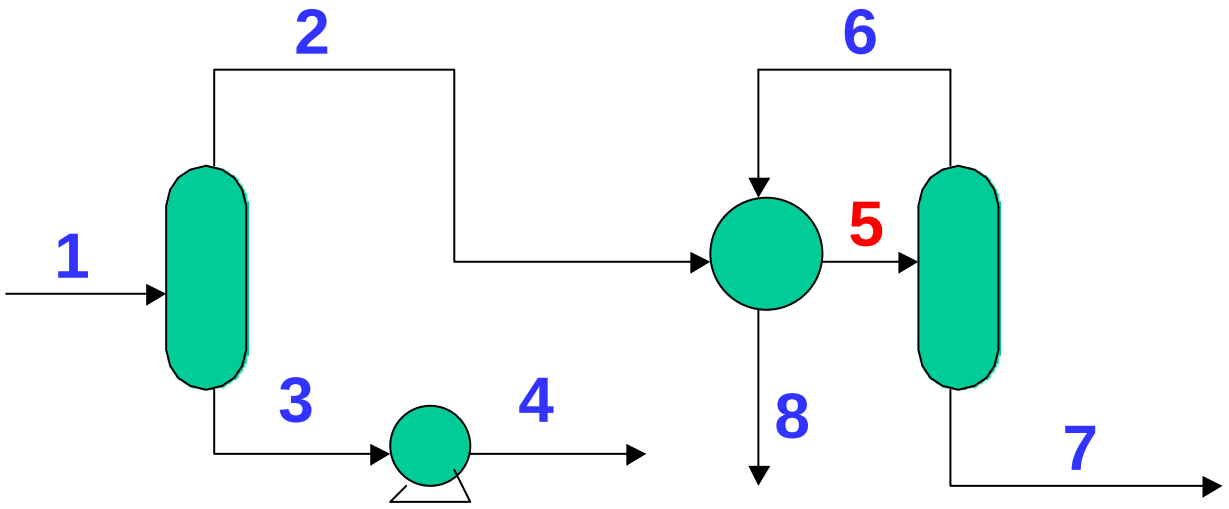
Buford D. Smith, 1963

공정 모사의 장점 (II)
Standardization

- Pure Component Database
  - 1,550개 가량의 순수성분 데이터베이스
  - (Commonly Used Components > 100)
- Binary Database
  - 10,000여 쌍의 이성분계에 대한 매개변수 내장
  - (100)x(100-1)/2 = 4950 BIP' s
- Thermodynamic Option
  - 60여 개의 열역학 모델식 내장
  - EOS Model, LACT Model, Special Package !

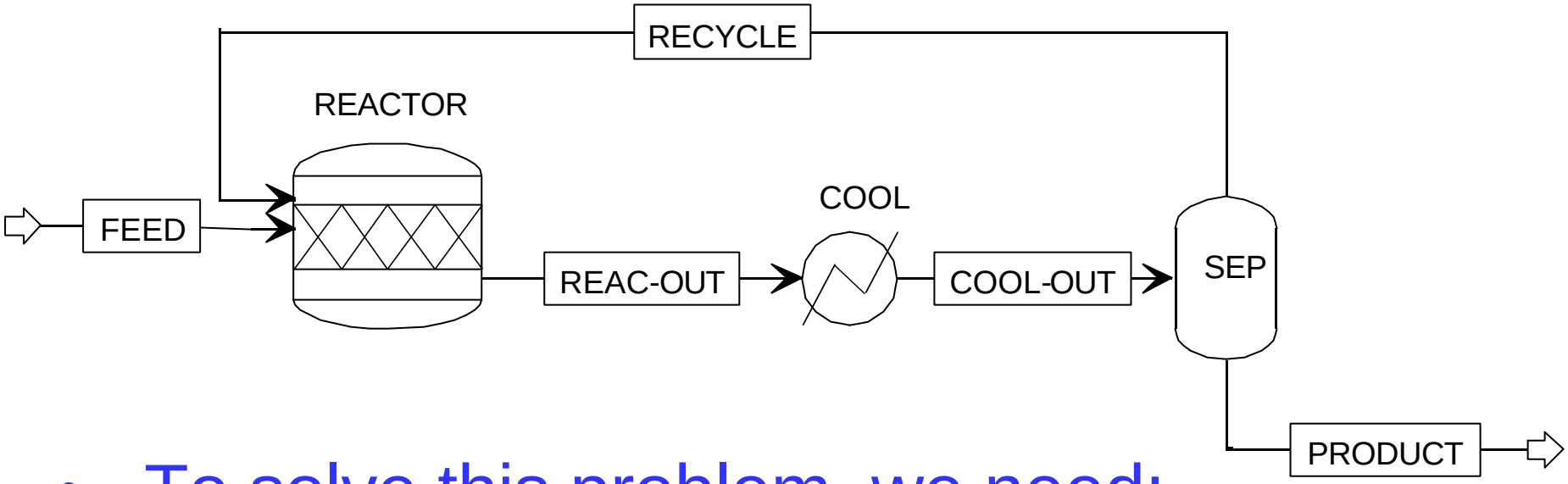
공정 모사의 장점 (III)
Solution of Recycle Process

- **Sequential-Modular Approach**



General Simulation Problem

What is the composition of stream PRODUCT?



- To solve this problem, we need:
  - Material balances
  - Energy balances

Approaches to Flowsheet Simulation

- Sequential Modular
  - Aspen Plus is a sequential modular simulation program.
  - Each unit operation block is solved in a certain sequence.
- Equation Oriented
  - Aspen Custom Modeler (formerly SPEEDUP) is an equation oriented simulation program.
  - All equations are solved simultaneously.
- Combination
  - Aspen Dynamics (formerly DynaPLUS) uses the Aspen Plus sequential modular approach to initialize the steady state simulation and the Aspen Custom Modeler (formerly SPEEDUP) equation oriented approach to solve the dynamic simulation.

Aspen Plus Basics

- The best way to learn Aspen Plus concepts is by using Aspen Plus. This session leads you through an example Aspen Plus simulation to explain how to open a file, enter data, run a simulation and examine results.

- It will allow one and half hour for this session.

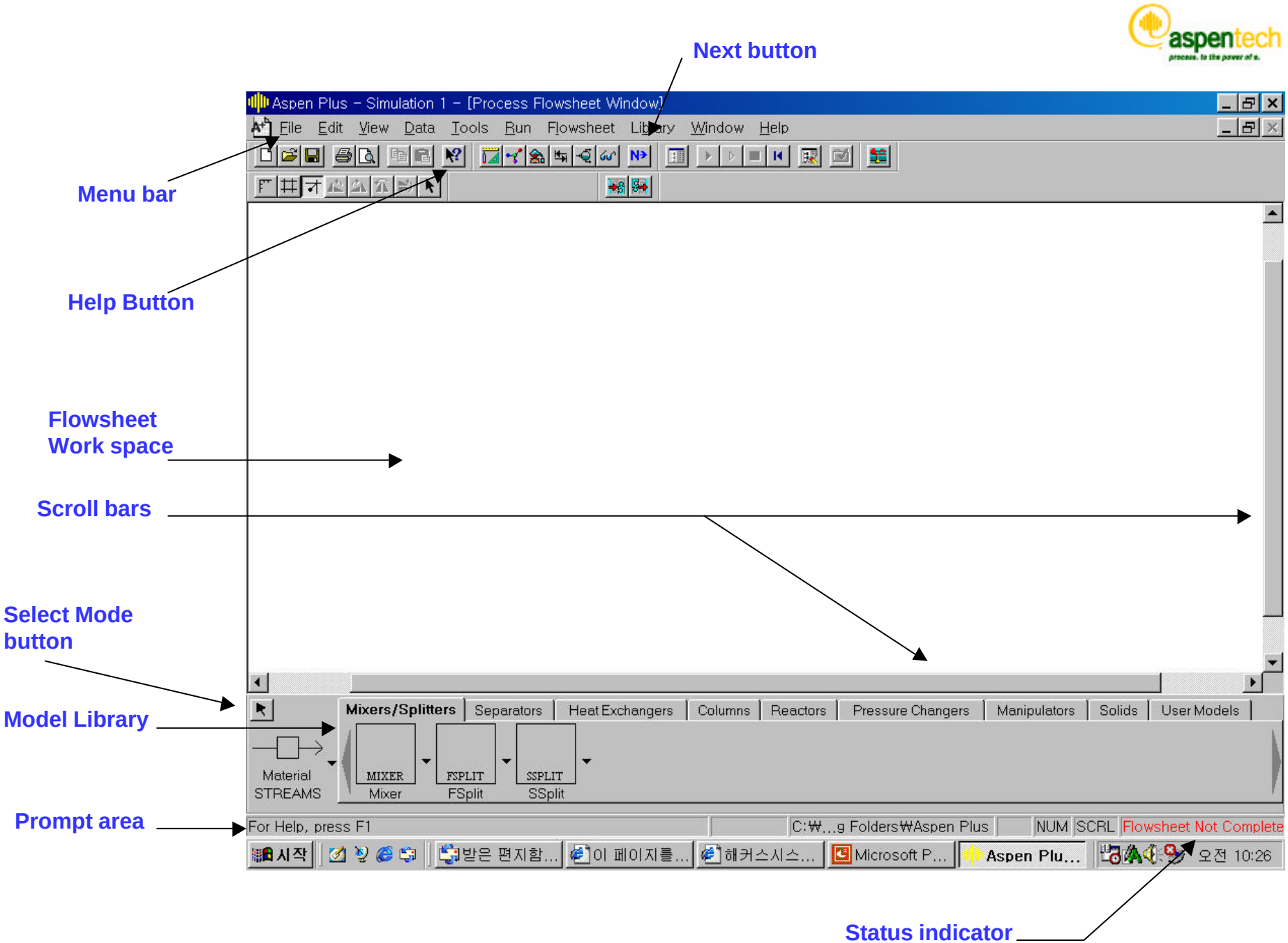
The User Interface

Objective:

Become comfortable and familiar with the Aspen Plus graphical user interface

Aspen Plus References:

- *User Guide*, Chapter 1, The User Interface
- *User Guide*, Chapter 2, Creating a Simulation Model
- *User Guide*, Chapter 4, Defining the Flowsheet


Next button
Menu bar
Help Button
Flowsheet
Work space
Scroll bars
Select Mode
button
Model Library
Prompt area
Status indicator
Aspen Plus – Simulation 1 – [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material
STREAMS
MIXER
Mixer
FSPLIT
FSplit
SSPLIT
SSplit
For Help, press F1
NUM
SCRL
Flowsheet Not Complete
시작
오전 10:26

Opening a File

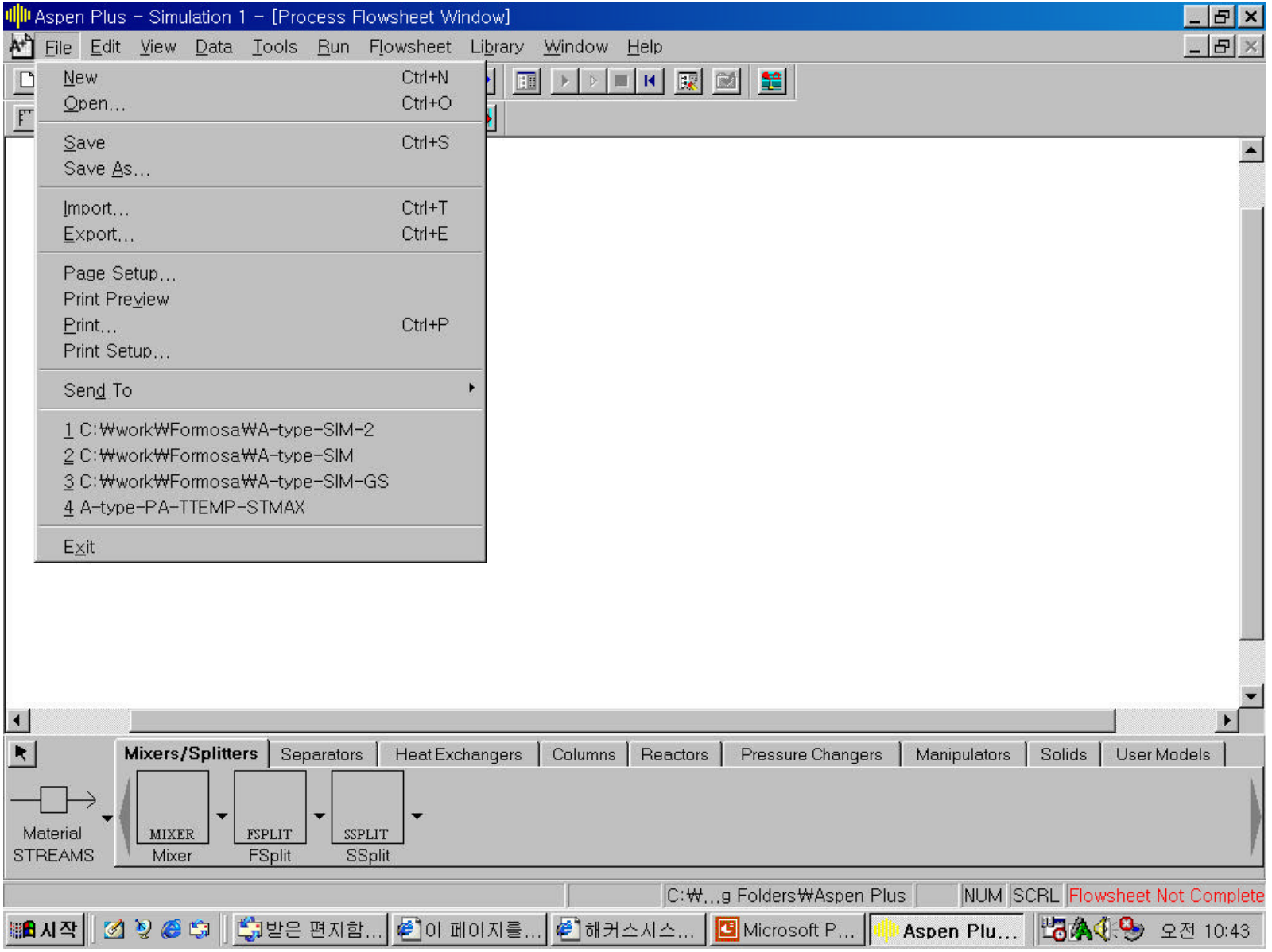
You can open a file for an Aspen Plus simulation by either:

- Double-clicking the file from Windows Explorer
- Selecting the open command from the File menu in Aspen Plus

In this session, you will use the open command on the File menu.

- To display the File menu, click File on the menu bar.

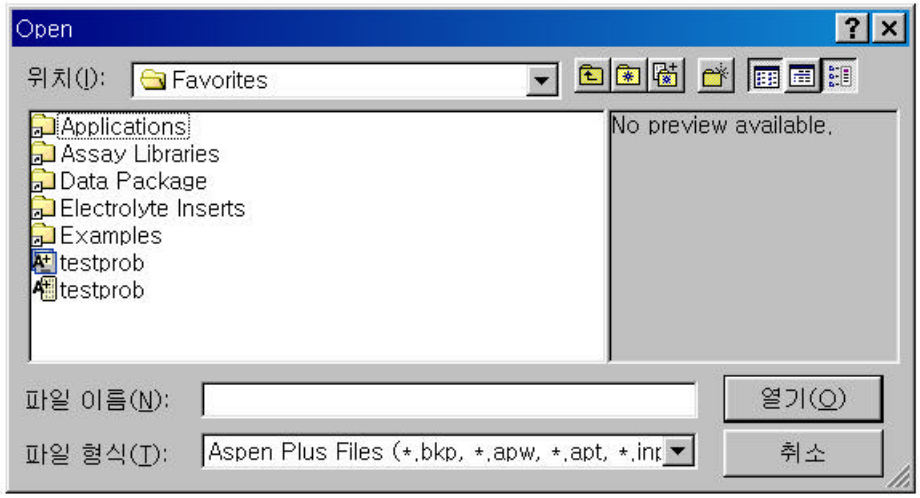
Aspen Plus displays the File menu:



- From the File menu, select Open.

  The Open dialog box appears. Your default working directory is displayed in the Look In box. You can navigate to the folder containing a file by using the Look In box or the Look In Favorite button,  .

- Click the Look in Favorite button.



Aspen Plus modeling Procedures

1. Define the process flowsheet modeled and the purpose of the model.
   (Setup Specifications Global) ***(Title Card in PRO/II)***
2. Select the units of measurement for input data and output.
3. Specify what chemical components will be present in the streams of the flowsheet.
   (Components Specifications Global) ***(Component Data in PRO/II)***
4. Specify the methods and models to be used for calculating physical properties.
   (Property Specifications Global) ***(Thermodynamic Data in PRO/II)***
5. Define the feed streams to the process.
   (Stream Specifications Global) ***(Stream Data in PRO/II)***
6. Convert the process flowsheet into unit operating blocks and choose an appropriate model for each block.
   (Block Specifications Global) ***(Unit Operations Data in PRO/II)***
7. Specify the performance of each unit operating block to represent the design and operating conditions of the process.
   (Design Specifications Global) ***(Specifications in PRO/II)***

Basic Input

The minimum required inputs (in addition to the graphical flowsheet) to run a simulation are:

- Setup	Title
- Components	Component Data
- Properties	Thermodynamic Data
- Streams	Stream Data
- Blocks	Unit Operations Data

Using the Mouse

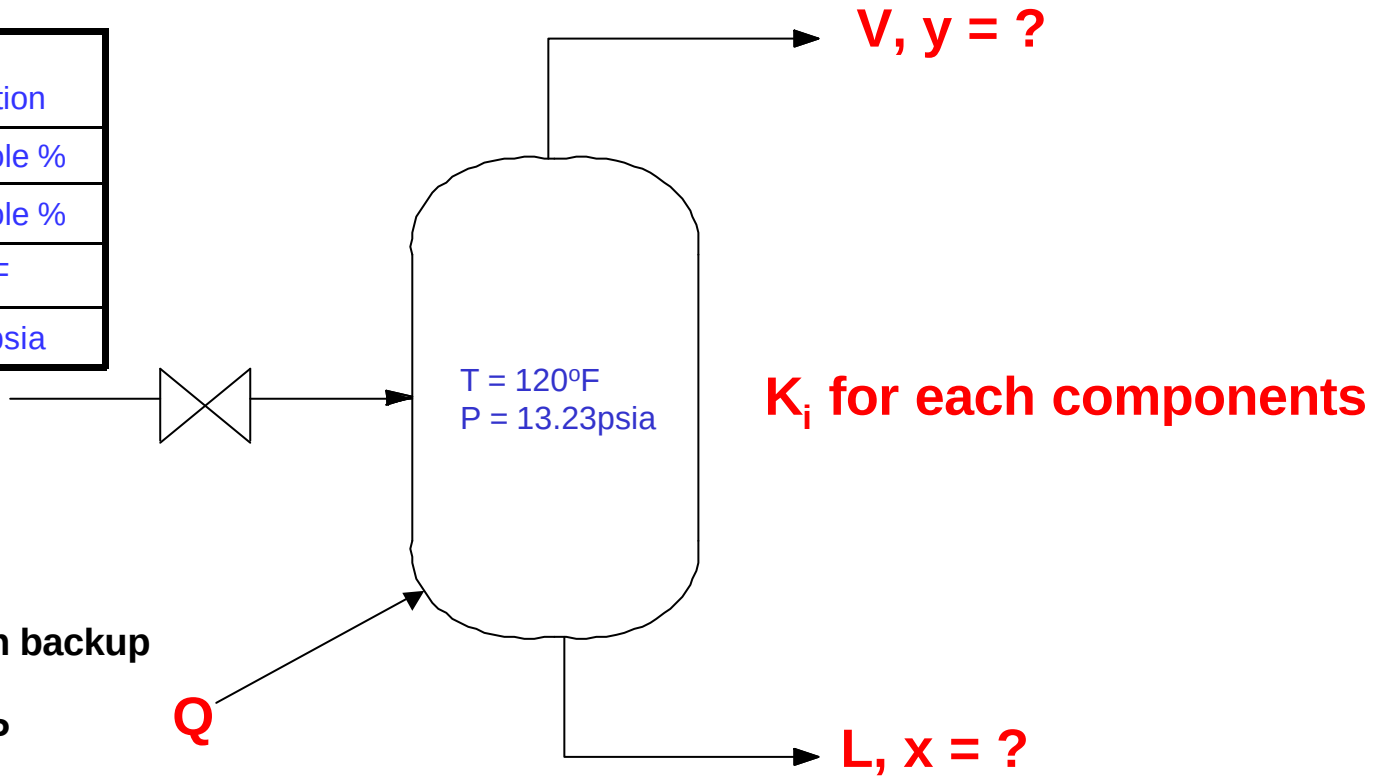
- Left button click - Select object/field
- Right button click - Bring up menu for selected object/field, or inlet/outlet
- Double left click - Open Data Browser object sheet

Reference: Aspen Plus User Guide, Chapter 1, The User Interface

Ex 1 : Two-phase Flash

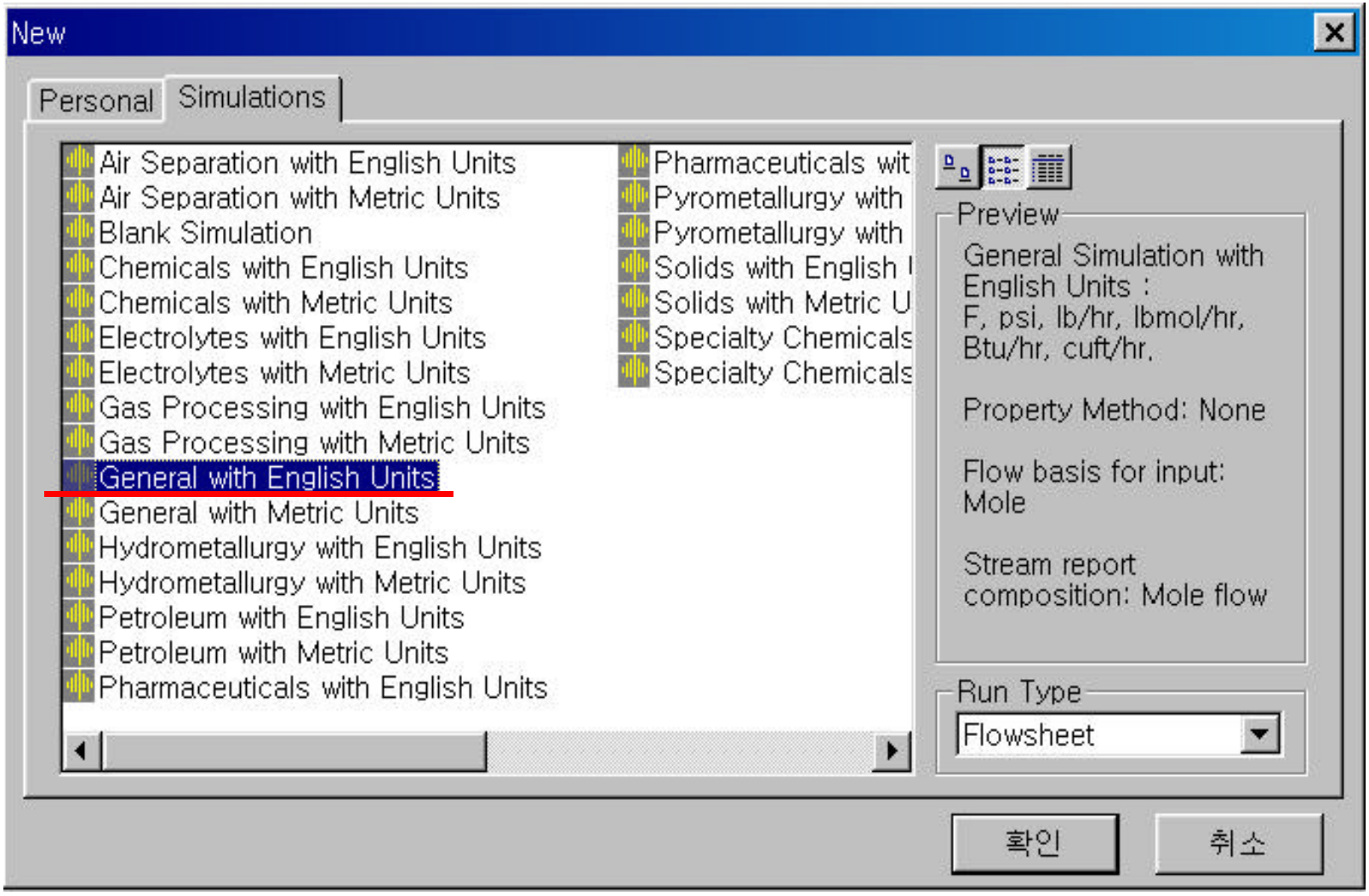
- An equimolar stream of *n*-pentane and *n*-hexane, at 130°F and 73.5 psia, is fed a flash vessel, where it is flashed to 13.23 psia with vapor liquid products in equilibrium at 120°F.
- Use ideal Raoulť s law for the simulation of this system.

Feed Characterization	
NC5	50 mole %
NC6	50 mole %
Temp.	130 °F
Press.	73.5 psia



When finished, save in backup format (Run-ID.BKP).
Filename: FLASH.BKP

Start with the General with English Units Template



Choose the appropriate icons for the block

- To place a block on the flowsheet:

1. Click on a model category tab in the Model Library.
2. Select a unit operation model. Click the drop-down arrow to select an icon for the model.
3. Click on the model and drag it to the flowsheet where you want to place the block, then release the mouse button.

Choose the appropriate icons for the block

- To place a stream on the flowsheet:

1. Click on the stream icon in the Model Library.
2. If you want to select a different stream type (Material, Heat or Work), click the down arrow next to the icon and choose a different type.
3. Click a highlighted port to make the connection.
4. Repeat step 3 to connect the other end of the stream.
5. To place one end of the stream as either a process flowsheet or product, click a blank part of the Process Flowsheet window.
6. Click the right mouse button on stop creating streams.

Graphic Flowsheet operations

- To display an input for a Block or a Stream in the Data Browser:

  1. Double click the left mouse on the object of interest.

- To rename, Delete, Change the icon, provide input or view results for a block or stream:

  1. Select object (Block or Stream) by clicking on it with the left mouse button.
  2. Click the right mouse while the pointer is over the selected object icon to bring up the menu for that object.
  3. Choose appropriate menu item.

Automatic Naming of Streams and Blocks

- Stream and block names can be automatically assigned by Aspen Plus or entered by the user when the object is created.

- Stream and block names can be displayed or hidden.
- To modify the naming options:

  - Select Options from the Tools menu.

  - Click the flowsheet tab.

  - Check or uncheck the naming options desired.

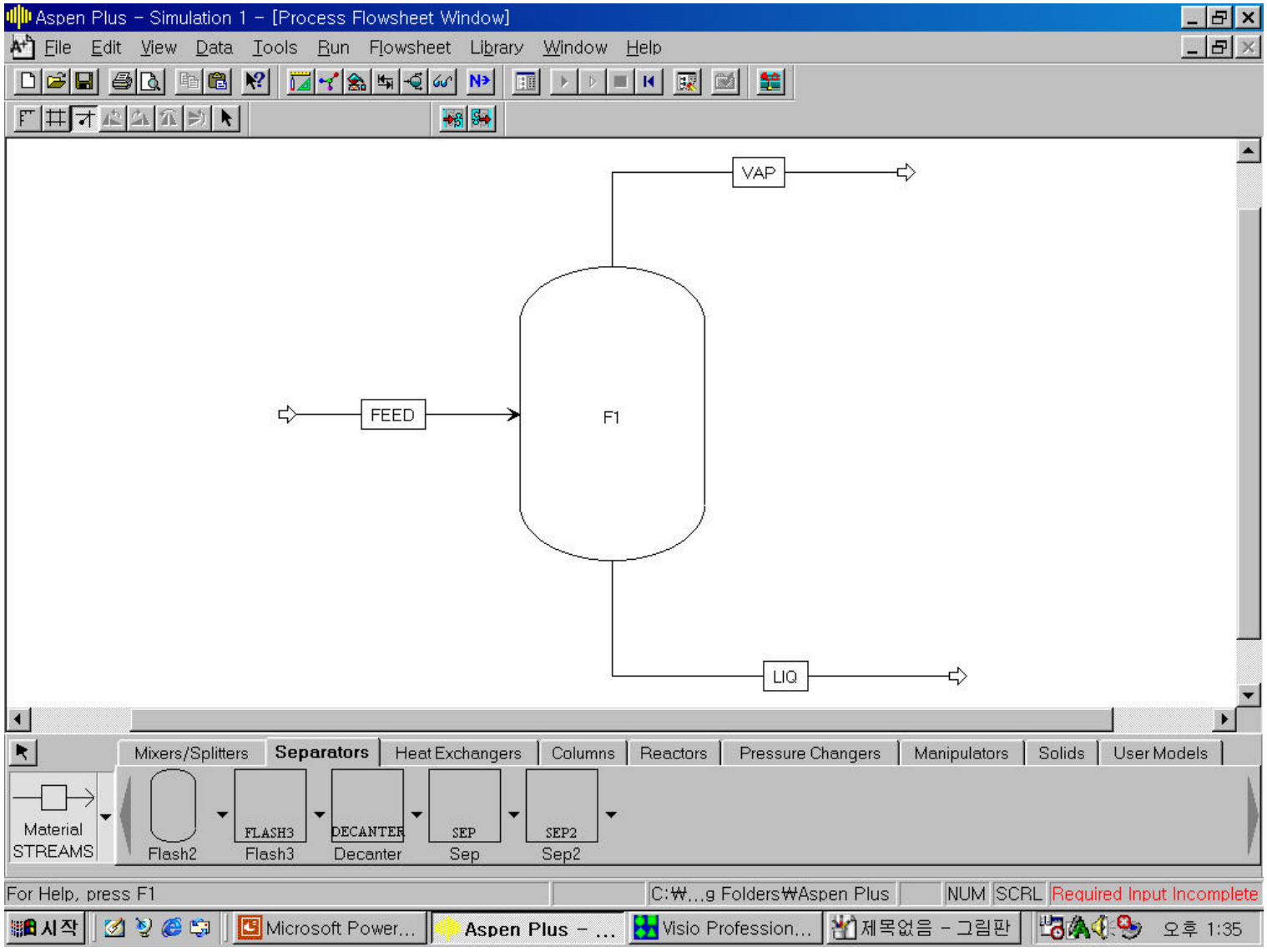
Setup

Most of the commonly used Setup information is entered on the *Setup Specifications Global* sheet:

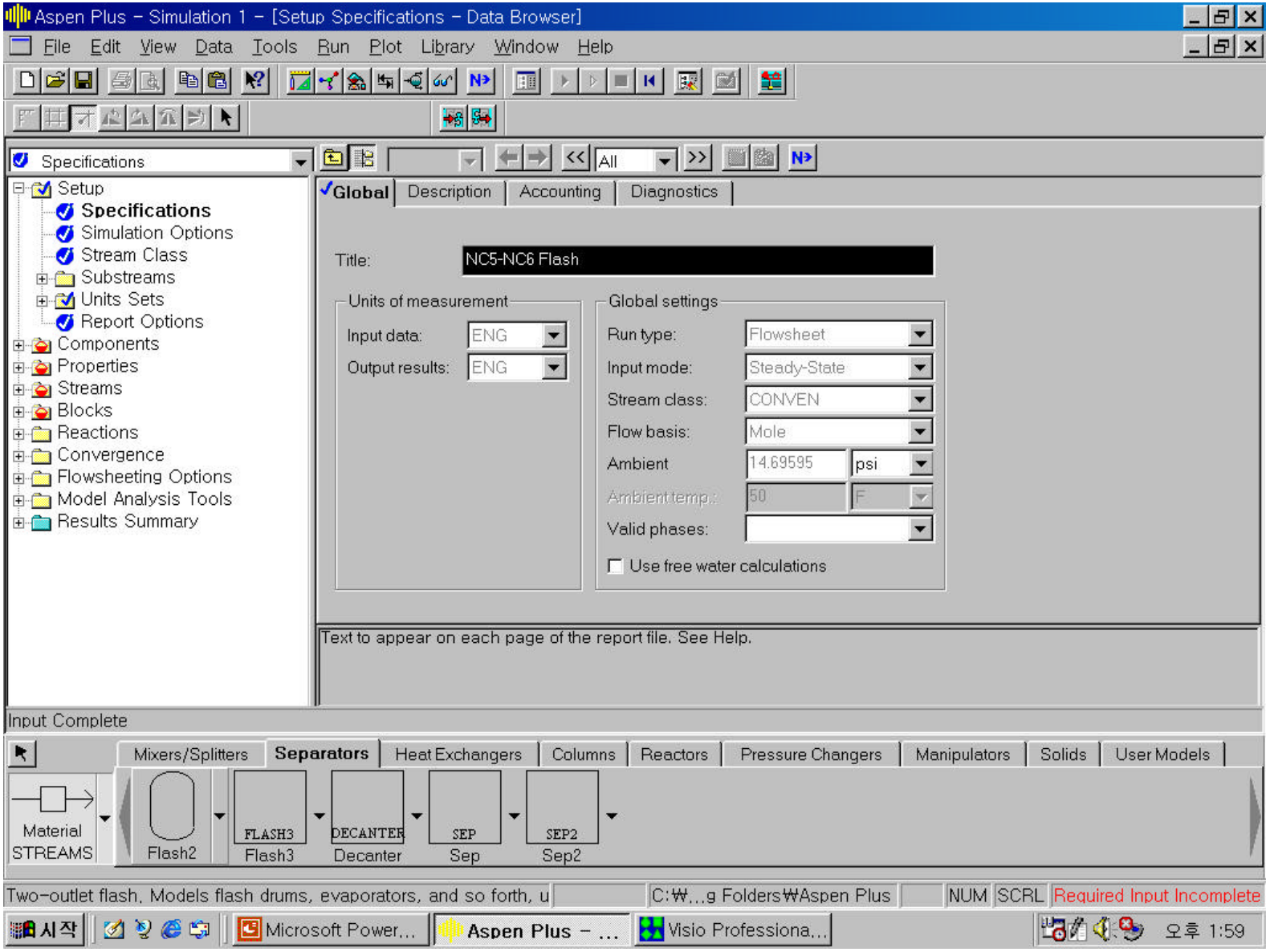
- Flowsheet title to be used on reports
- Run type
- Input and output units
- Valid phases (e.g. vapor-liquid or vapor-liquid-liquid)
- Ambient pressure

Stream report options are located on the *Setup Report Options Stream* sheet.

Step 1 : general process information (Setup Specifications)



Step 1 : general process information (Setup Specifications) ***continued***



Status Indicators

Symbol	Status
	Input for the form is incomplete
	Input for the form is complete
	No input for the form has been entered. It is optional.
	Results for the form exist.
	Results for the form exist, but there were calculation errors.
	Results for the form exist, but there were calculation warnings.
	Results for the form exist, but input has changed since the results were generated.

Setup Run Types

Run Type	
Flowsheet	Standard Aspen Plus flowsheet run including sensitivity studies and optimization. Flowsheet runs can contain property estimation, assay data analysis, and/or property analysis calculations.
Assay Data Analysis	A standalone Assay Data Analysis and pseudocomponent generation run Use Assay Data Analysis to analyze assay data when you do not want to perform a flowsheet simulation in the same run.
Data Regression	A standalone Data Regression run Use Data Regression to fit physical property model parameters required by ASPEN PLUS to measured pure component, VLE, LLE, and other mixture data. Data Regression can contain property estimation and property analysis calculations. ASPEN PLUS cannot perform data regression in a Flowsheet run.
PROPERTIES PLUS	PROPERTIES PLUS setup run Use PROPERTIES PLUS to prepare a property package for use with Aspen Custom Modeler (formerly SPEEDUP) or Aspen Pinch (formerly ADVENT), with third-party commercial engineering programs, or with your company's in-house programs. You must be licensed to use PROPERTIES PLUS.
Property Analysis	A standalone Property Analysis run Use Property Analysis to generate property tables, PT-envelopes, residue curve maps, and other property reports when you do not want to perform a flowsheet simulation in the same run. Property Analysis can contain property estimation and assay data analysis calculations.
Property Estimation	Standalone Property Constant Estimation run Use Property Estimation to estimate property parameters when you do not want to perform a flowsheet simulation in the same run.

Setup Units

- Units in Aspen Plus can be defined at 3 different levels:
  1. Global Level ("Input Data" & "Output Results" fields on the *Setup Specifications Global* sheet)
  2. Object level ("Units" field in the top of any input form

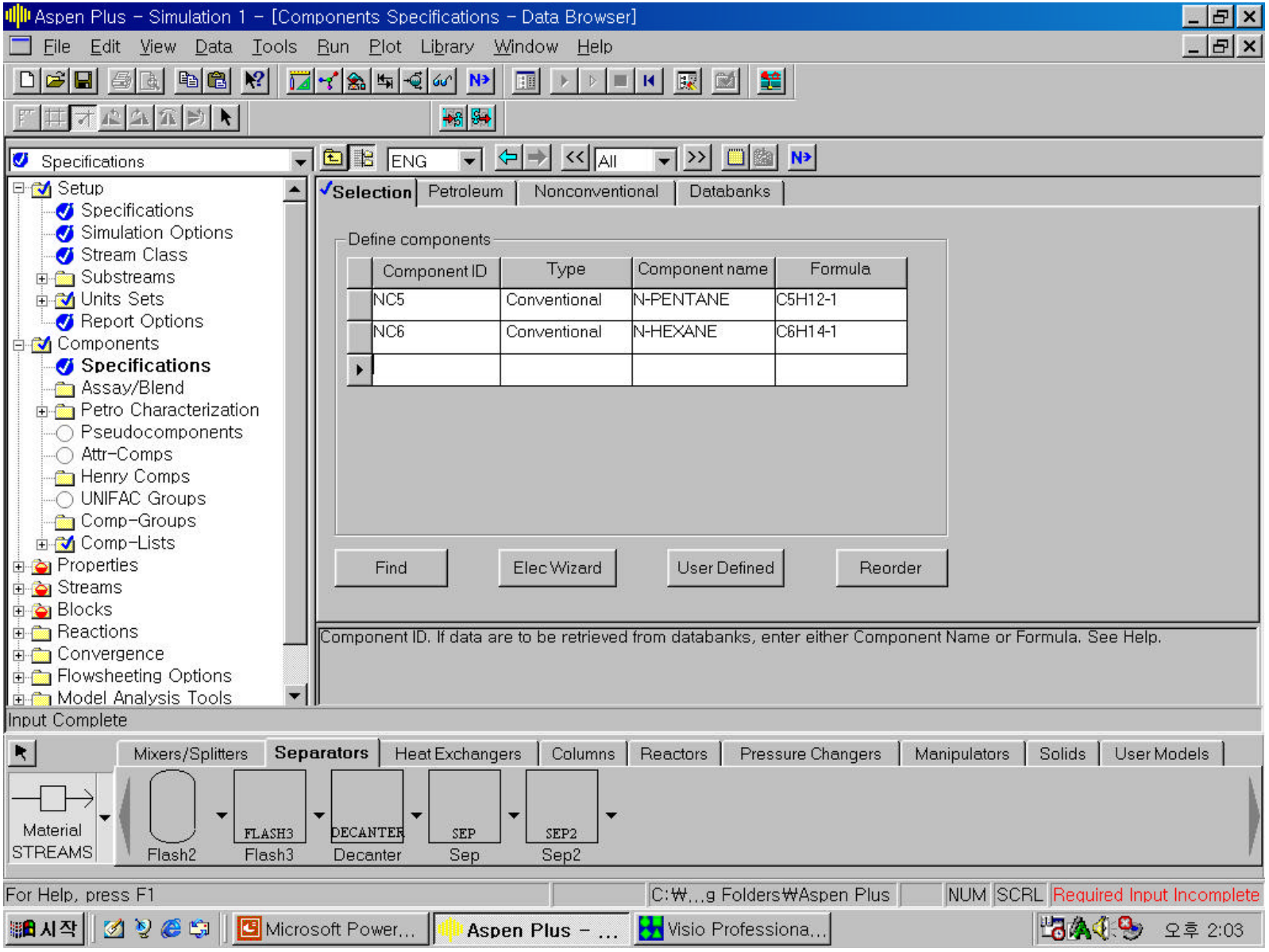
     of an object such as a block or stream
  3. Field Level

- Users can create their own units sets using the *Setup Units Sets* Object Manager. Units can be copied from an existing set and then modified.

Components

- Use the *Components Specifications* form to specify all the components required for the simulation.
- If available, physical property parameters for each component are retrieved from databanks.
- Pure component databanks contain parameters such as molecular weight, critical properties, etc. The databank search order is specified on the Databanks sheet.
- The Find button can be used to search for components.
- The Electrolyte Wizard can be used to set up an electrolyte simulation.

Step 2 : chemical species (Component Specifications Form)



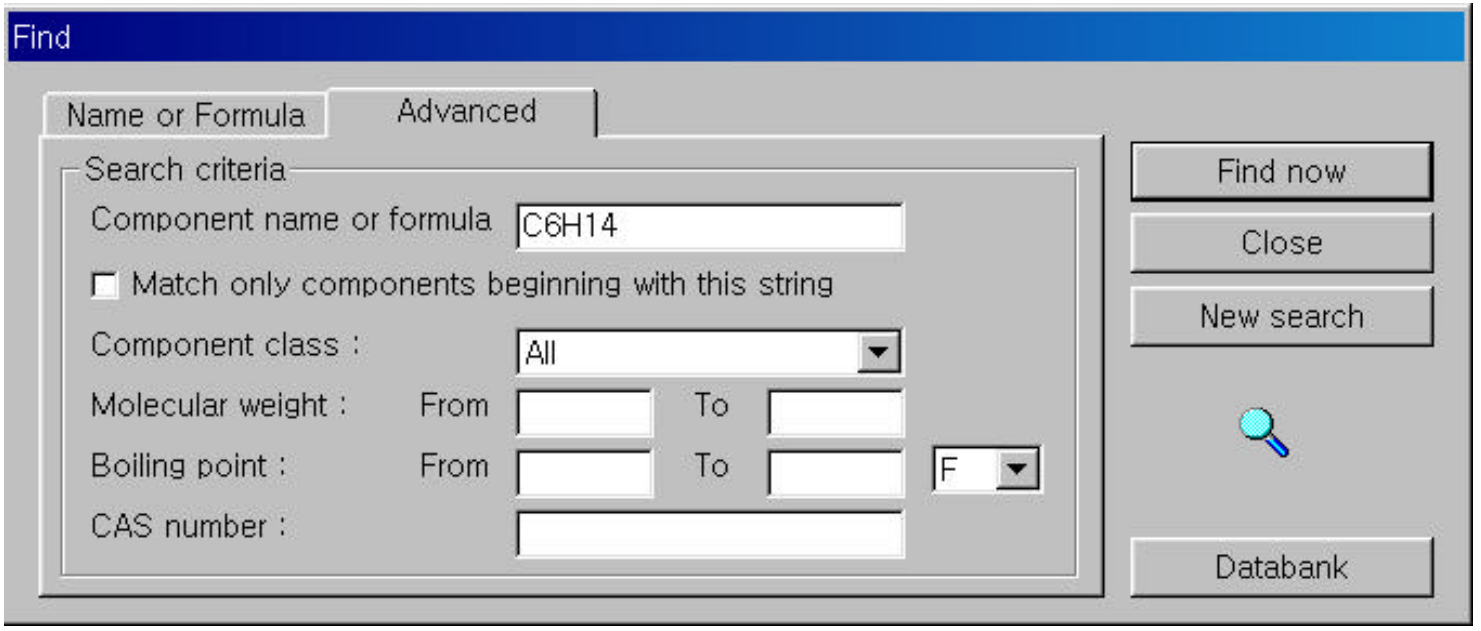
Entering Components

- The Component ID is used to identify the component in simulation inputs and results.
- Each Component ID can be associated with a databank component as either:

  - Formula: Chemical formula of component (e.g., C6H6)
  (Note that a suffix is added to formulas when there are isomers, e.g. C2H6O-2)
  - Component Name: Full name of component (e.g., BENZENE)

- Databank components can be searched for using the Find button.
  - Search using component name, formula, component class, molecular weight, boiling point, pr CAS number.
  - All components containing specified items will be listed.

Find



- Find performs an AND search when more than one criterion is specified.

Pure Component Databanks

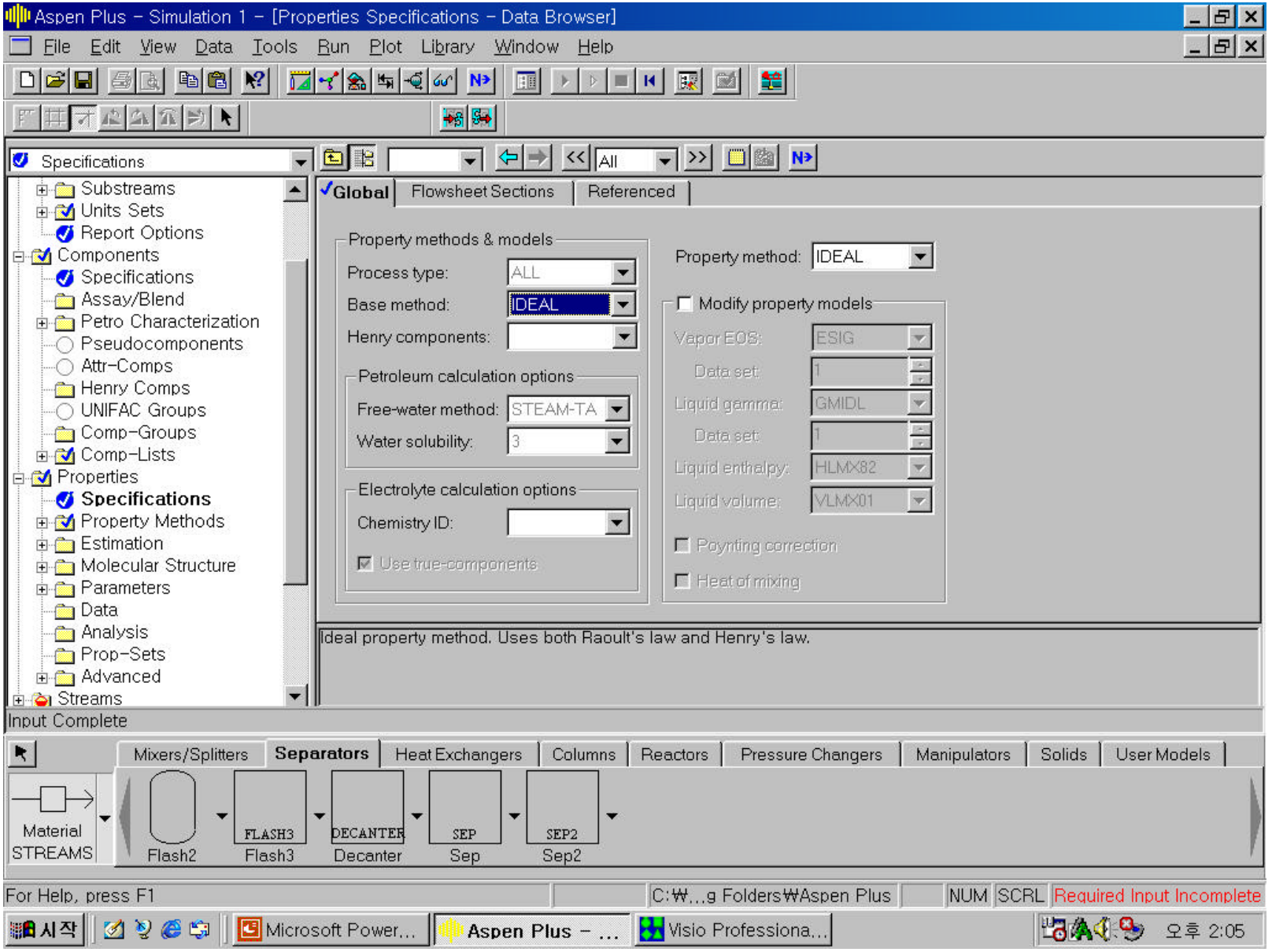
Databank	Contents	Use
PURE10	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech	Primary component databank in Aspen Plus
AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
INORGANIC	Thermochemical properties for inorganic components in vapor, liquid and solid states	Solids, electrolytes, and metallurgy applications
PURE93	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech delivered with Aspen Plus 9.3	For upward compatibility
PURE856	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech delivered with Aspen Plus 8.5-6	For upward compatibility

Parameters missing from the first selected databanks will be searched for in subsequent selected databanks.

Properties

- Use the *Properties Specifications* form to specify the physical property methods to be used in the simulation.
- Property methods are a collection of models and methods used to describe pure component and mixture behavior.
- Choosing the right physical properties is critical for obtaining reliable simulation results.
- Selecting a Process Type will narrow the number of methods available.

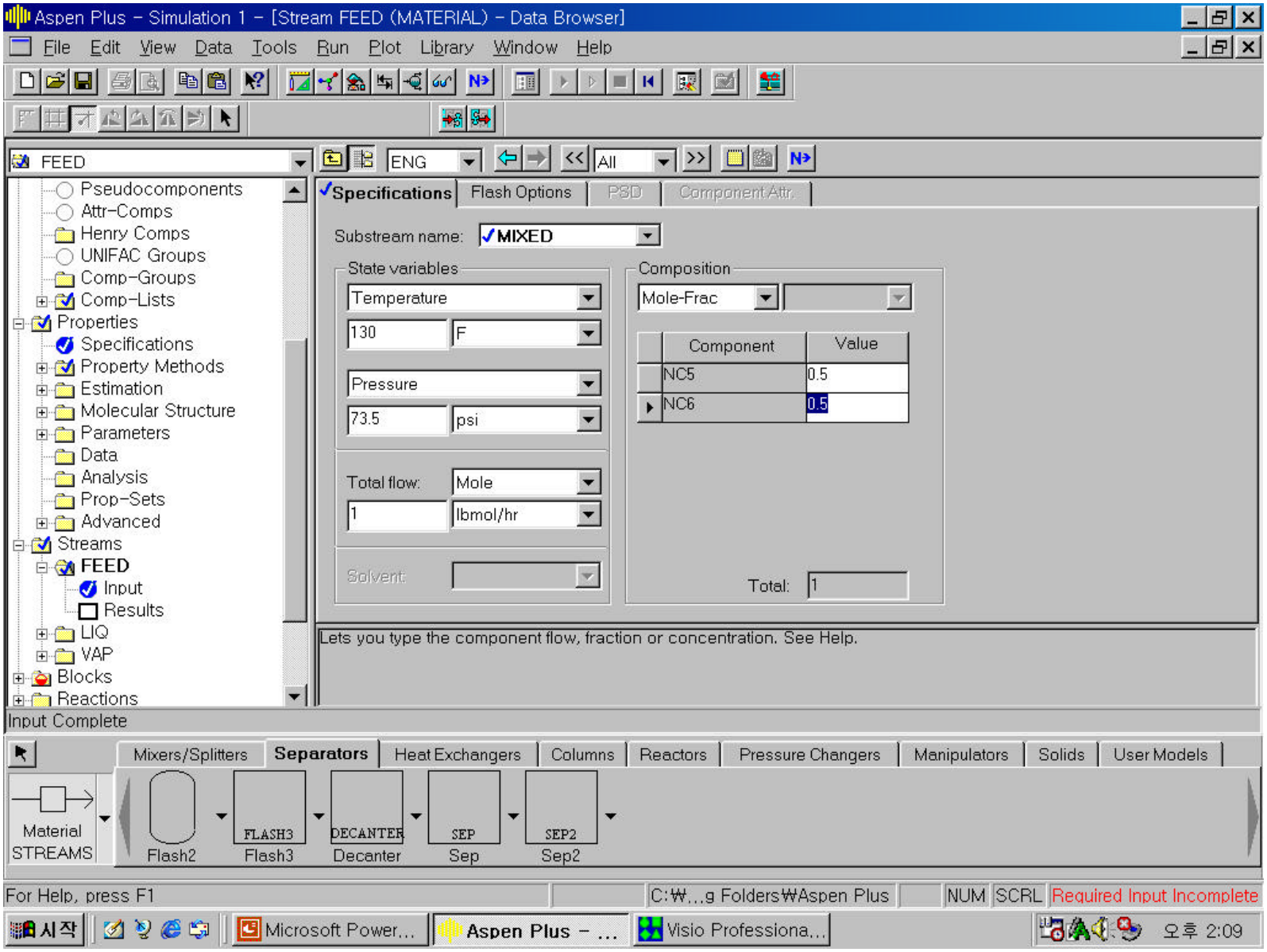
Step 3 : physical property (Property Specifications Global Form)



Streams

- Use *Stream Input* forms to specify the feed stream conditions and composition.
- To specify stream conditions enter two of the following:
  - Temperature
  - Pressure
  - Vapor Fraction
- To specify stream composition enter either:
  - Total stream flow and component fractions
  - Individual component flows
- Specifications for streams that are not feeds to the flowsheet (i.e. recycle streams) are used as estimates.

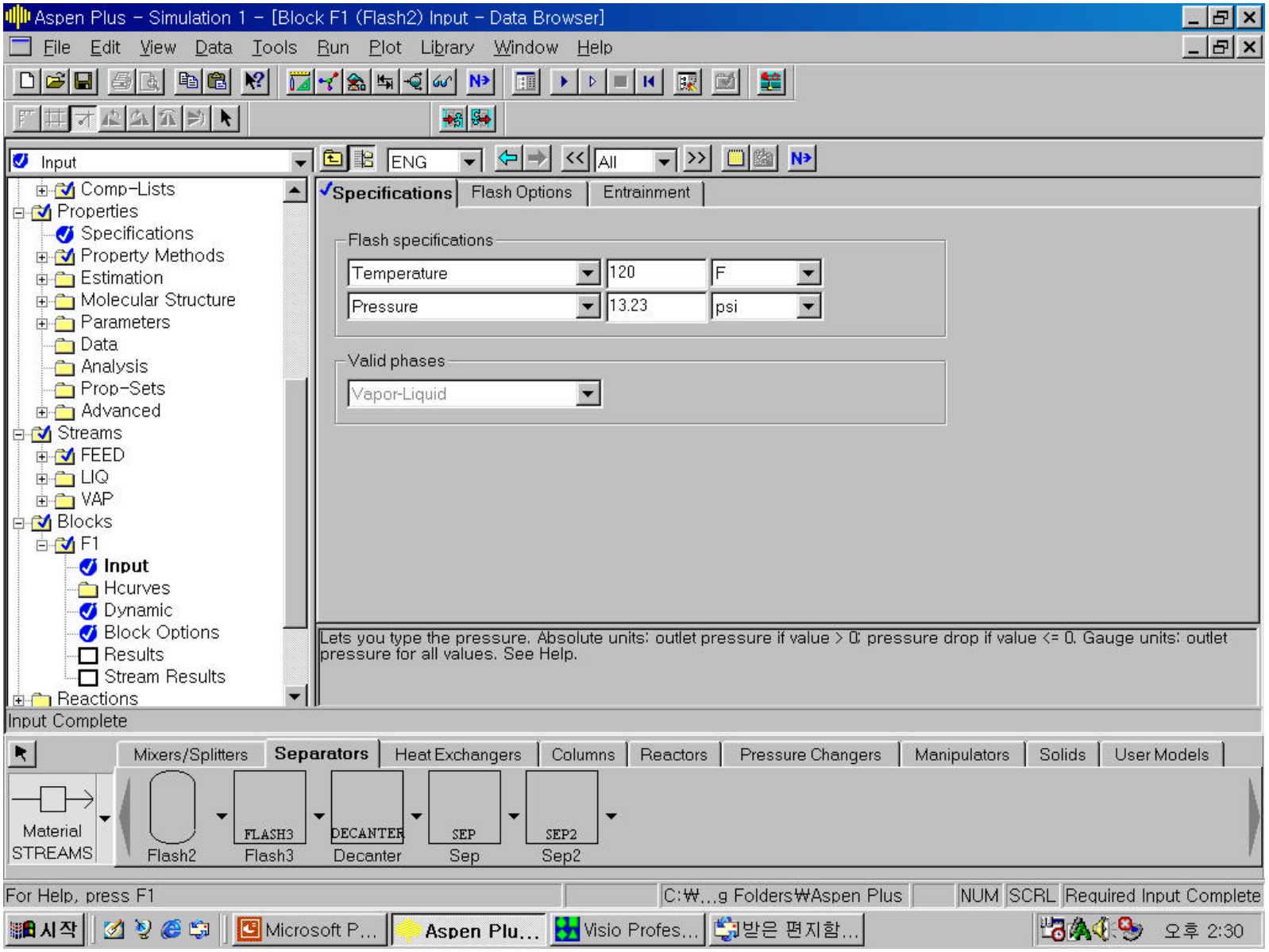
Step 4 : stream variables (Stream Specifications form)



Blocks

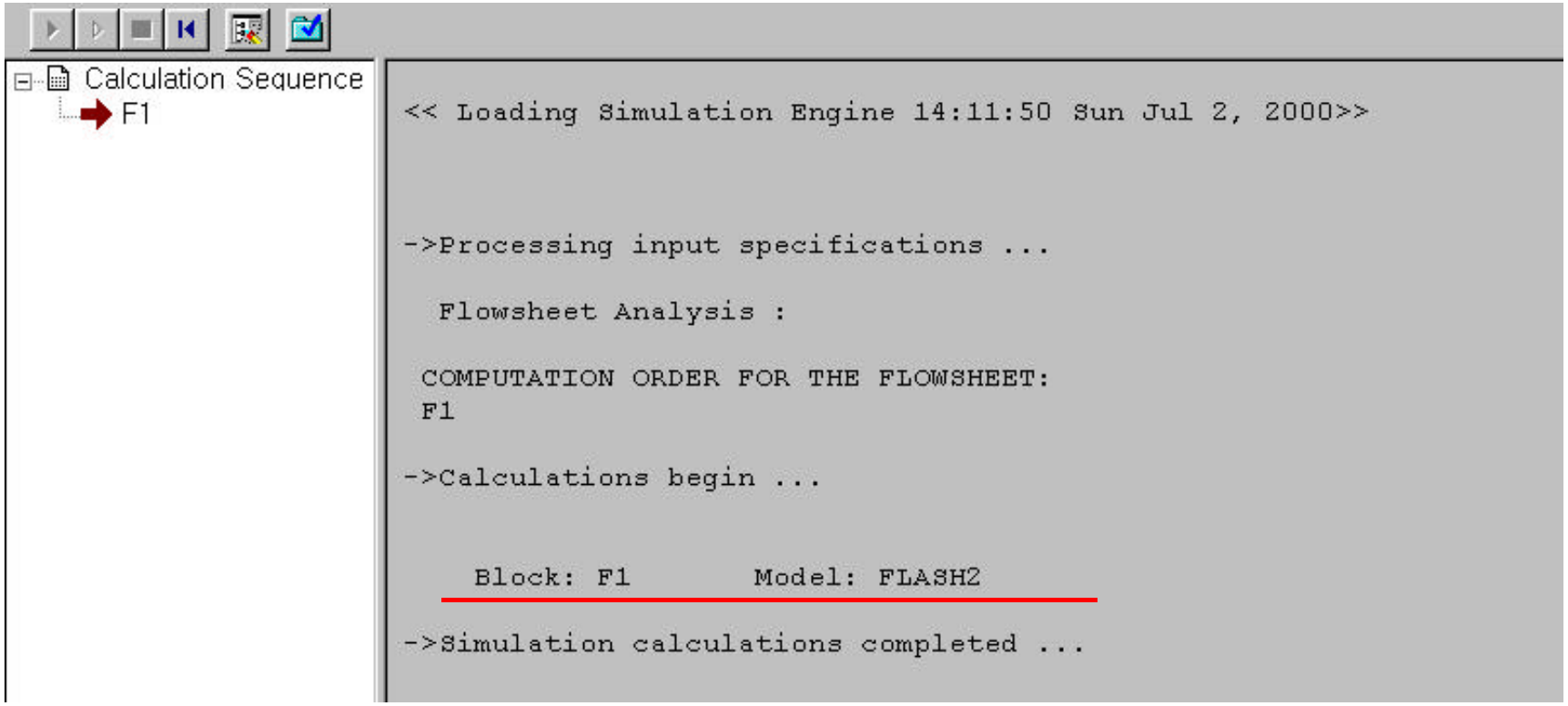
- Each *Block Input* or *Block Setup* form specifies operating conditions and equipment specifications for the unit operation model.
- Some unit operation models require additional specification forms
- All unit operation models have optional information forms (e.g. *BlockOptions* form).

Step 5 : equipment parameters (Block [Flash2] Specifications Form)



Starting the Run

- Select *Control Panel* from the *View* menu or press the Next button to be prompted.
  - The simulation can be executed when all required forms are complete.
  - The Next button will take you to any incomplete forms.



Control Panel

The Control Panel consists of:

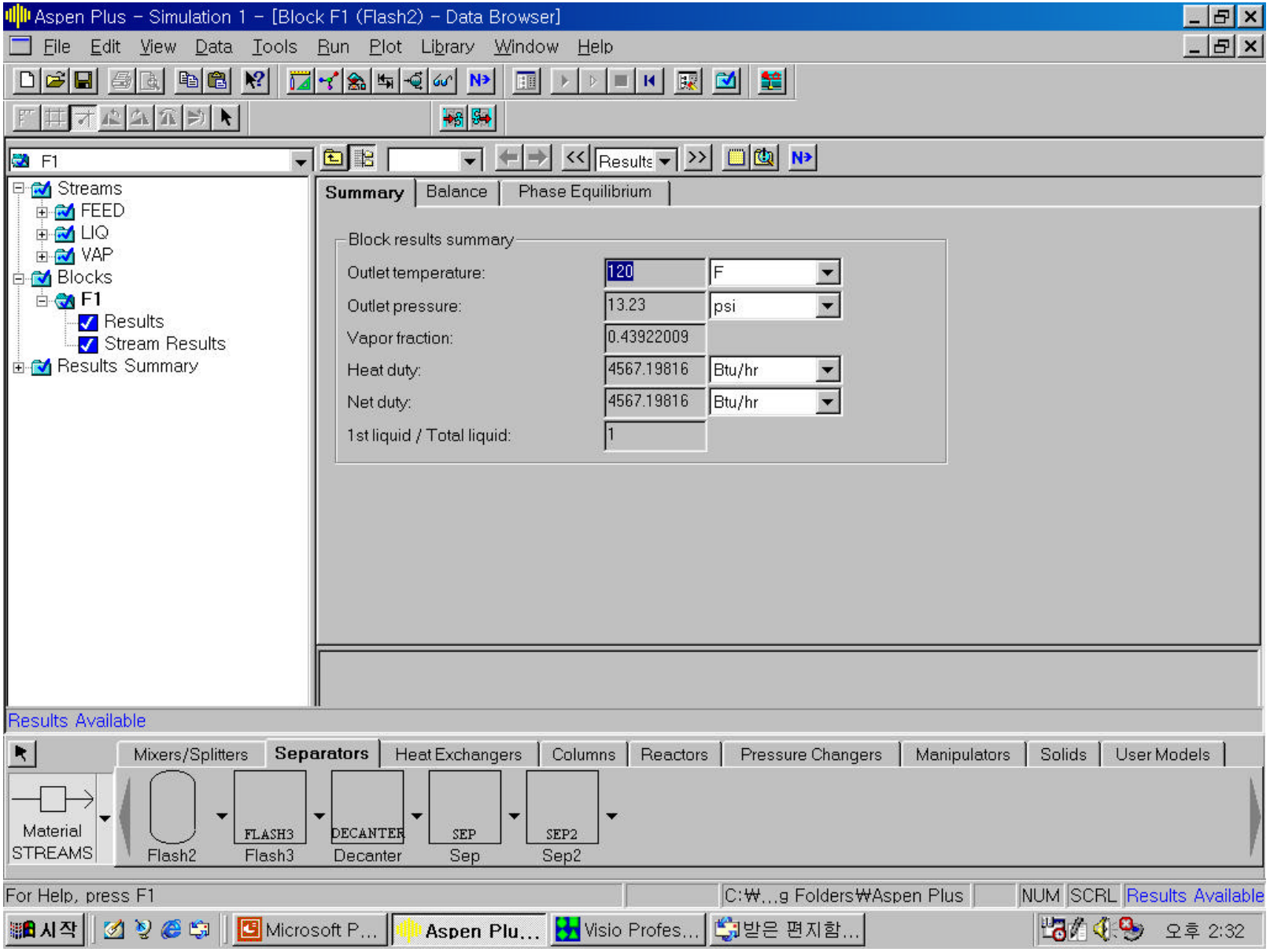
- A message window showing the progress of the simulation by displaying the most recent messages from the calculations
- A status area showing the hierarchy and order of simulation blocks and convergence loops executed
- A toolbar which you can use to control the simulation

Run		Start or continue calculations
Step		Step through the flowsheet one block at a time
Stop		Pause simulation calculations
Reinitialize		Purge simulation results
Results		Check simulation results

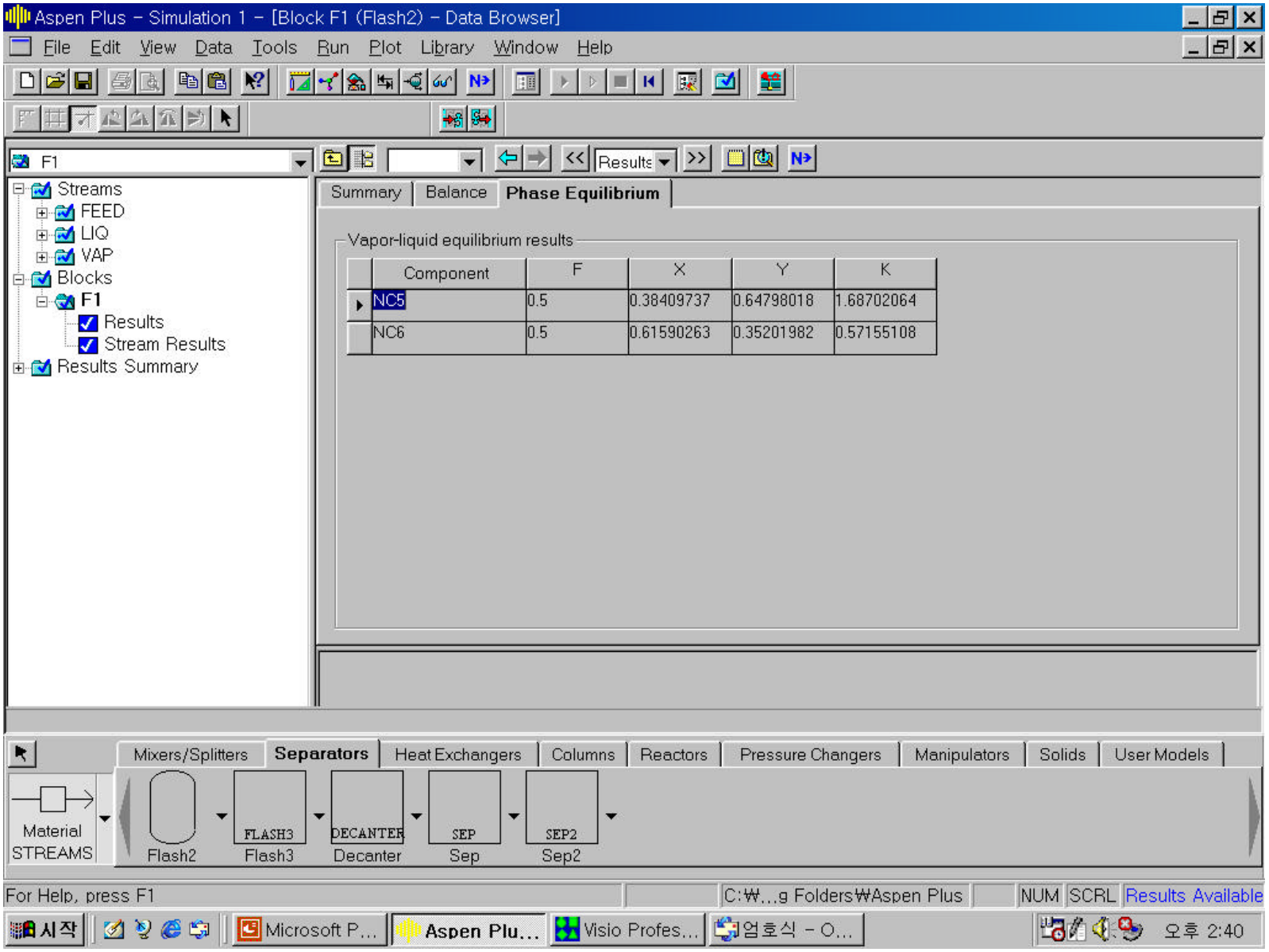
Reviewing Results

- History file or Control Panel Messages
  - Contains any generated errors or warnings
  - Select *History* or *Control Panel* on the *View* menu to display the History file or the Control Panel
- Stream Results
  - Contains stream conditions and compositions
    - For all streams *(/Data/Results Summary/Streams)*
    - For individual streams (bring up the stream folder in the Data Browser and select the *Results* form)
- Block Results
  - Contains calculated block operating conditions *(*bring up the block folder in the Data Browser and select the *Results* form*)*

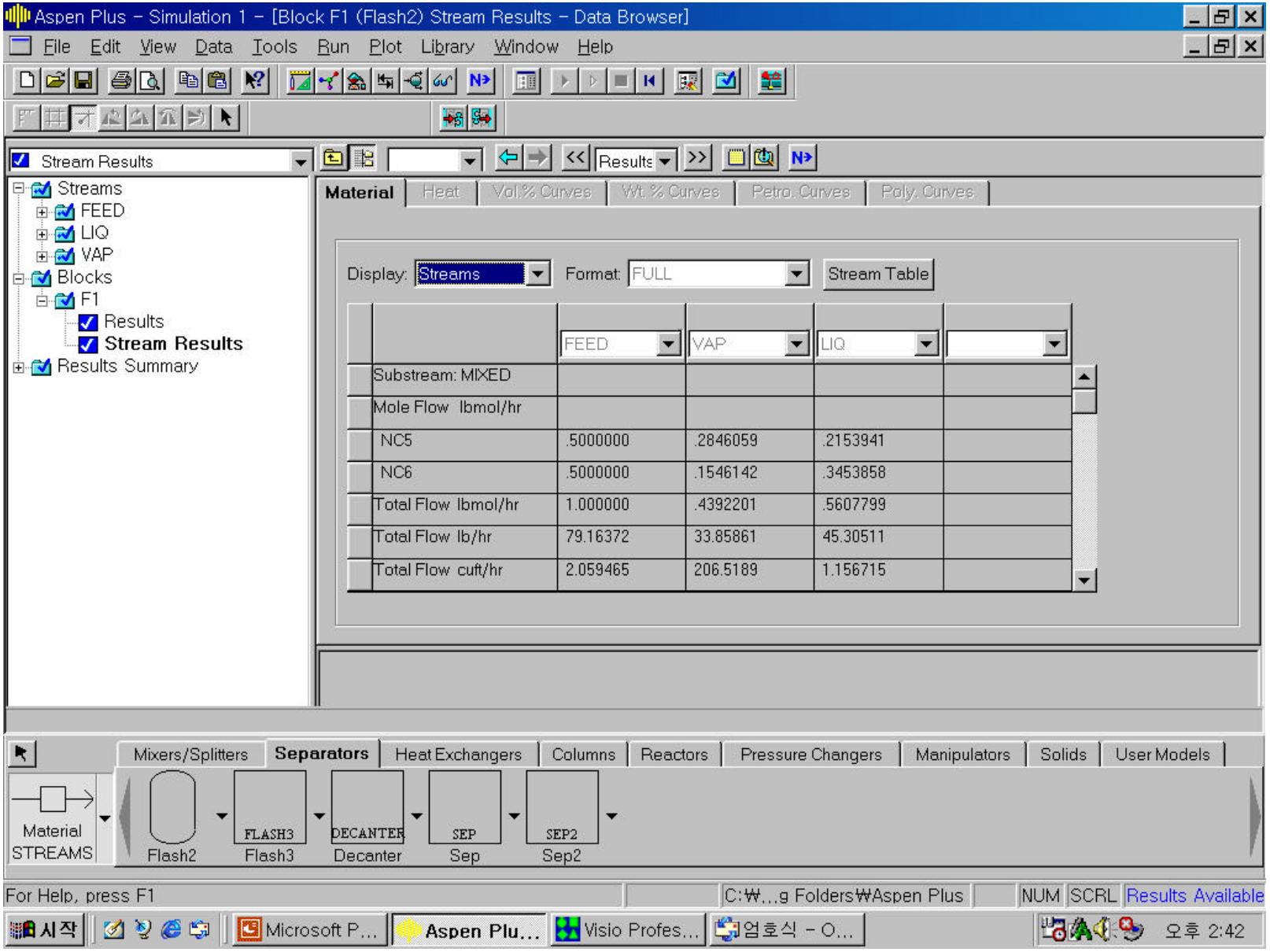
Examine result 1 : Aspen Plus Output



Examine results : Aspen Plus Output - *continued*



Examine results : Aspen Plus Output - *continued*



Unit Operation Models

- ***Objective:***

  Review major types of unit operation models

Aspen Plus References:

- *User Guide*, Chapter 10, Unit Operation Models
- *Unit Operation Models Reference Manual*

Unit Operation Model Types

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

Mixers/Splitters

Model	Description	Purpose	Use
Mixer	Stream mixer	Combine multiple streams into one stream	Mixing tees, stream mixing operations, adding heat streams, adding work streams
FSplit	Stream splitter	Split stream flows	Stream splitters, bleed valves
SSplit	Substream splitter	Split substream flows	Solid stream splitters, bleed valves

Separators

Model	Description	Purpose	Use
Flash2	Two-outlet flash	Determine thermal and phase conditions	Flashes, evaporators, knockout drums, single stage separators
Flash3	Three-outlet flash	Determine thermal and phase conditions	Decanters, single stage separators with two liquid phases
Decanter	Liquid-liquid decanter	Determine thermal and phase conditions	Decanters, single stage separators with two liquid phases and no vapor phase
Sep	Multi-outlet component separator	Separate inlet stream components into any number of outlet streams	Component separation operations such as distillation and absorption, when the details of the separation are unknown or unimportant
Sep2	Two-outlet component separator	Separate inlet stream components into two outlet streams	Component separation operations such as distillation and absorption, when the details of the separation are unknown or unimportant

Heat Exchangers

Model	Description	Purpose	Use
Heater	Heater or cooler	Determines thermal and phase conditions	Heaters, coolers, valves. Pumps and compressors when work-related results are not needed.
HeatX	Two-stream heat exchanger	Exchange heat between two streams	Two-stream heat exchangers. Rating shell and tube heat exchangers when geometry is known.
MHeatX	Multistream heat exchanger	Exchange heat between any number of streams	Multiple hot and cold stream heat exchangers. Two-stream heat exchangers. LNG exchangers.
Hetran*	Interface to B-JAC Hetran program	Design and simulate shell and tube heat exchangers	Shell and tube heat exchangers with a wide variety of configurations.
Aerotran*	Interface to B-JAC Aerotran program	Design and simulate air-cooled heat exchangers	Air-cooled heat exchangers with a wide variety of configurations. Model economizers and the convection section of fired heaters.

Columns - Shortcut

Model	Description	Purpose	Use
DSTWU	Shortcut distillation design	Determine minimum RR, minimum stages, and either actual RR or actual stages by Winn-Underwood-Gilliland method.	Columns with one feed and two product streams
Distl	Shortcut distillation rating	Determine separation based on RR, stages, and D:F ratio using Edmister method.	Columns with one feed and two product streams
SCFrac	Shortcut distillation for petroleum fractionation	Determine product composition and flow, stages per section, duty using fractionation indices.	Complex columns, such as crude units and vacuum towers

Columns - Rigorous

Model	Description	Purpose	Use
RadFrac	Rigorous fractionation	Rigorous rating and design for single columns	Distillation, absorbers, strippers, extractive and azeotropic distillation, reactive distillation
MultiFrac	Rigorous fractionation for complex columns	Rigorous rating and design for multiple columns of any complexity	Heat integrated columns, air separators, absorber/stripper combinations, ethylene primary fractionator/quench tower combinations, petroleum refining
PetroFrac	Petroleum refining fractionation	Rigorous rating and design for petroleum refining applications	Preflash tower, atmospheric crude unit, vacuum unit, catalytic cracker or coker fractionator, vacuum lube fractionator, ethylene fractionator and quench towers
BatchFrac*+	Rigorous batch distillation	Rigorous rating calculations for single batch columns	Ordinary azeotropic batch distillation, 3-phase, and reactive batch distillation
RateFrac*	Rate-based distillation	Rigorous rating and design for single and multiple columns. Based on nonequilibrium calculations	Distillation columns, absorbers, strippers, reactive systems, heat integrated units, petroleum applications
Extract	Liquid-liquid extraction	Rigorous rating for liquid-liquid extraction columns	Liquid-liquid extraction

* Requires separate license and + Input language only in version 10.0

Reactors

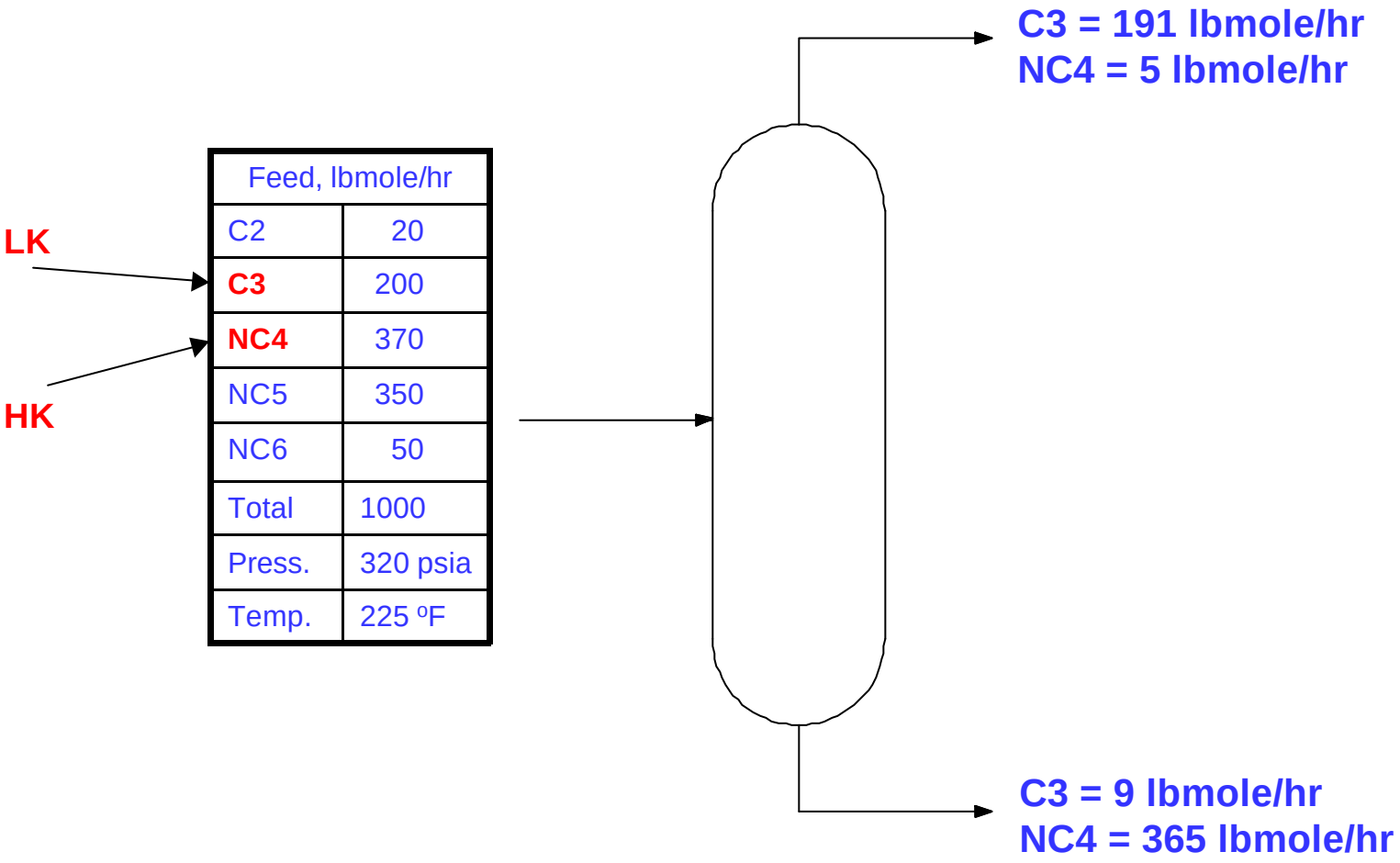
Model	Description		Purpose	Use
RStoic	Stoichiometric reactor		Stoichiometric reactor with specified reaction extent or conversion	Reactors where the kinetics are unknown or unimportant but stoichiometry and extent are known
RYield	Yield reactor		Reactor with specified yield	Reactors where the stoichiometry and kinetics are unknown or unimportant but yield distribution is known
REquil	Equilibrium reactor		Chemical and phase equilibrium by stoichiometric calculations	Single- and two-phase chemical equilibrium and simultaneous phase equilibrium
RGibbs	Equilibrium reactor		Chemical and phase equilibrium by Gibbs energy minimization	Chemical and/or simultaneous phase and chemical equilibrium. Includes solid phase equilibrium.
RCSTR	Continuous stirred tank reactor		Continuous stirred tank reactor	One, two, or three-phase stirred tank reactors with kinetics reactions in the vapor or liquid
RPlug	Plug flow reactor		Plug flow reactor	One, two, or three-phase plug flow reactors with kinetic reactions in any phase. Plug flow reactions with external coolant.
RBatch	Batch reactor		Batch or semi-batch reactor	Batch and semi-batch reactors where the reaction kinetics are known

Pressure Changers

Model	Description	Purpose	Use
Pump	Pump or hydraulic turbine	Change stream pressure when the pressure, power requirement or performance curve is known	Pumps and hydraulic turbines
Compr	Compressor or turbine	Change stream pressure when the pressure, power requirement or performance curve is known	Polytropic compressors, polytropic positive displacement compressors, isentropic compressors, isentropic turbines.
MCompr	Multi-stage compressor or turbine	Change stream pressure across multiple stages with intercoolers. Allows for liquid knockout streams from intercoolers	Multistage polytropic compressors, polytropic positive compressors, isentropic compressors, isentropic turbines.
Valve	Control valve	Determine pressure drop or valve coefficient (CV)	Multi-phase, adiabatic flow in ball, globe and butterfly valves
Pipe	Single-segment pipe	Determine pressure drop and heat transfer in single-segment pipe or annular space	Multi-phase, one dimensional, steady-state and fully developed pipeline flow with fittings
Pipeline	Multi-segment pipe	Determine pressure drop and heat transfer in multi-segment pipe or annular space	Multi-phase, one dimensional, steady-state and fully developed pipeline flow

Ex 2 : Hydrocarbon Distillation

- For the simulation of a depropanizer that involves five normal paraffins: ethane through *n*-hexane.



Depropanizer New Design

1. Determine the number of tray to obtain:
   a) C3 recovery at overhead : 99.5 %
   b) NC4 recovery at overhead : 1.35 %

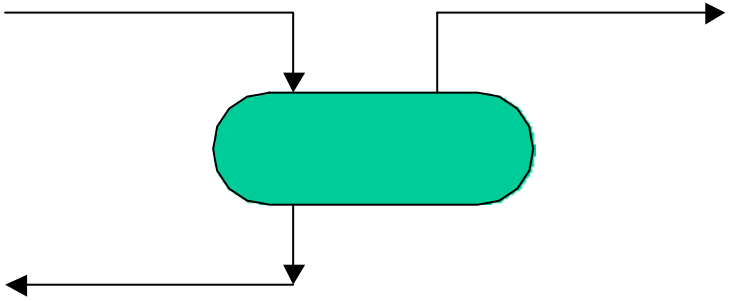
2. Determine the column pressure, based on a dew point condenser temperature of 130^{o}F.

3. Use RK-Soave (SRK in PRO/II) method for VLE calculation.

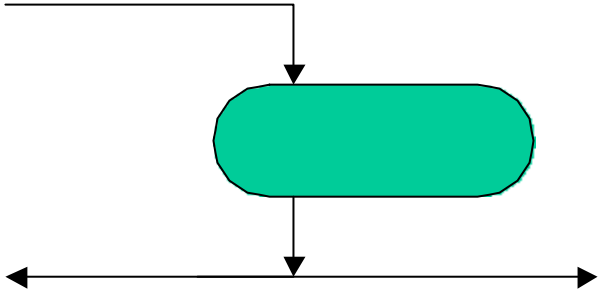
4. Find an actual reflux ratio which minimizes the summation of total utility consumptions *(operating costs)* and theoretical number of stages *(capital costs)*.

How we can determine the condenser type?
or How we can determine the column pressure?

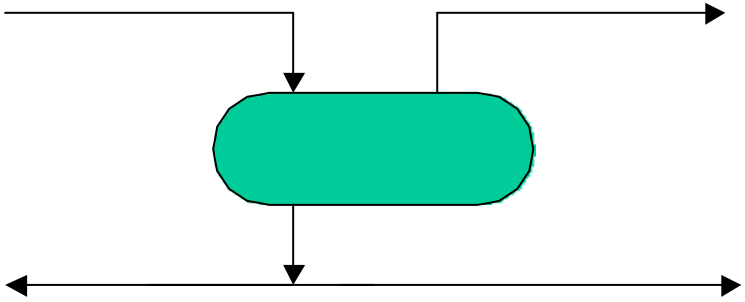
A. Partial



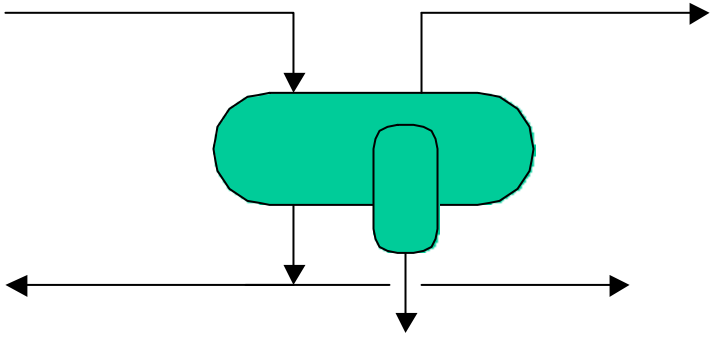
B. Bubble or sub-cooled



C. Mixed



D. Mixed with decanter



It depends on the refrigerant available and overhead compositions to be assumed.

- Overhead molar flow rate (assume)

  C2 = 30, C3 = 191, NC4 = 5

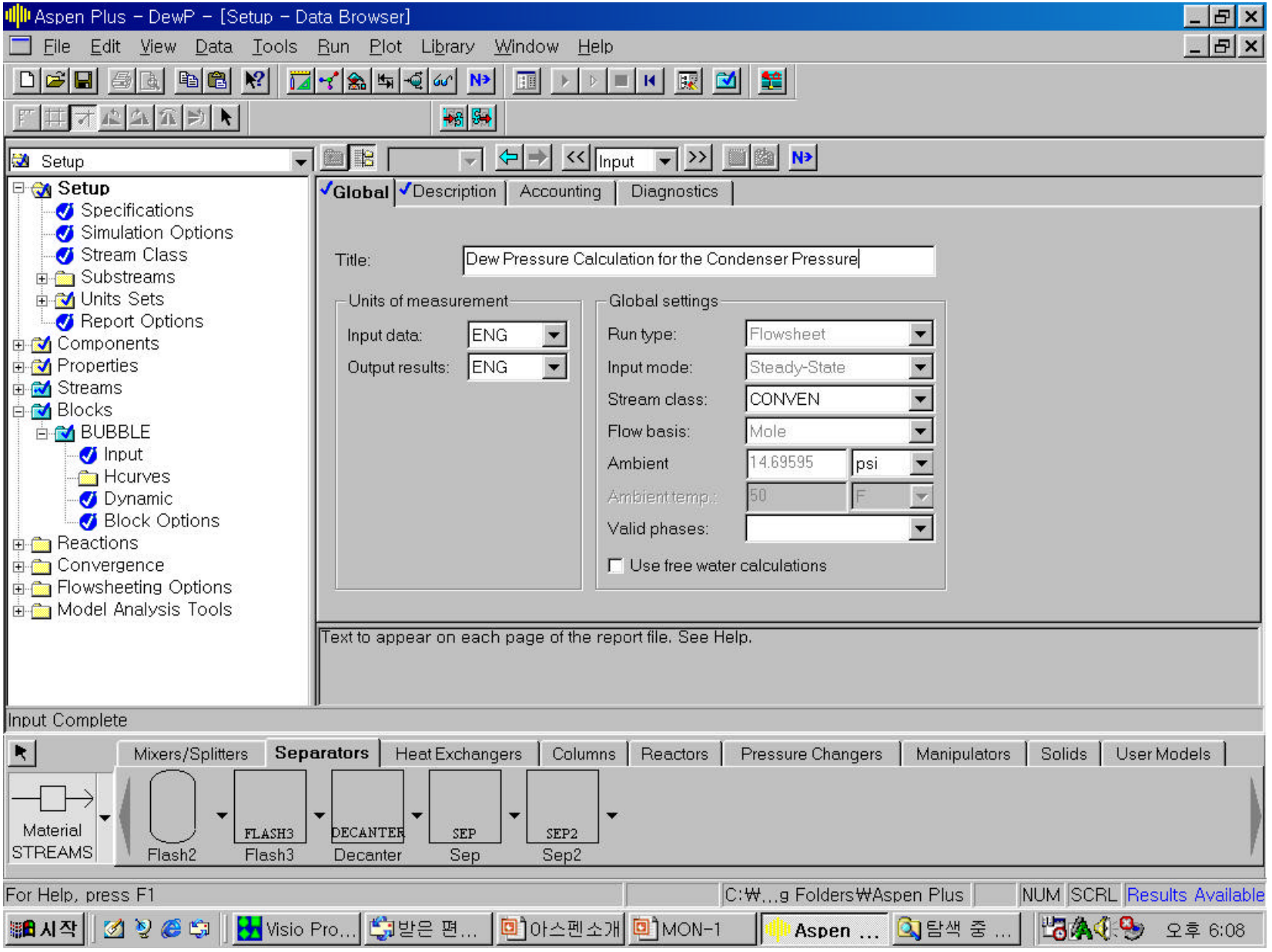
- Normalize ! (Component mole %)

  C2 = 13.27, C3 = 84.51, NC4 = 2.22

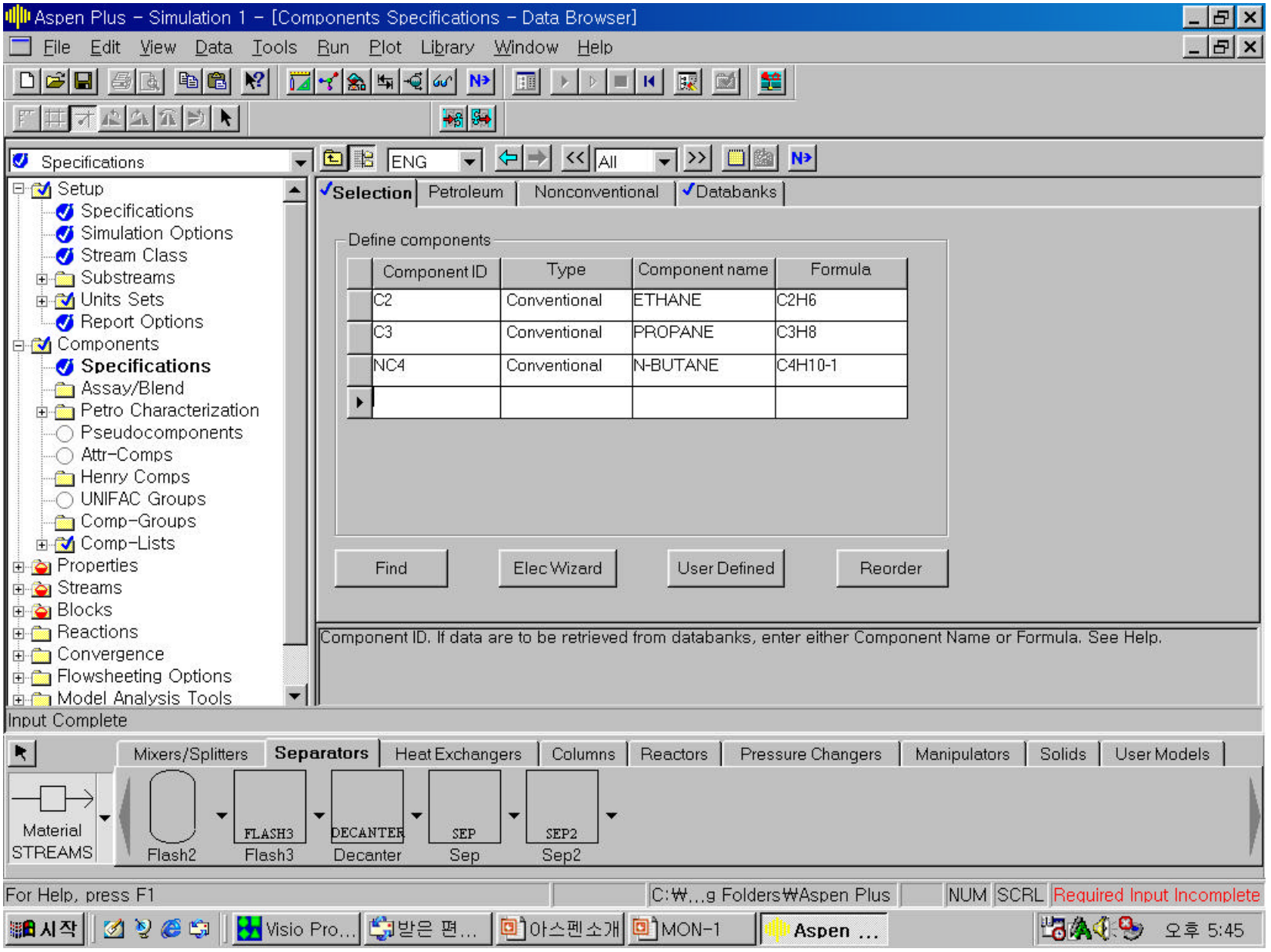
- First, we have to determine the dew point pressure !

Component	Mole %
C2	13.27
C3	84.51
NC4	2.22
Temperature (°F)	130.00
Dew P at 130 °F	?

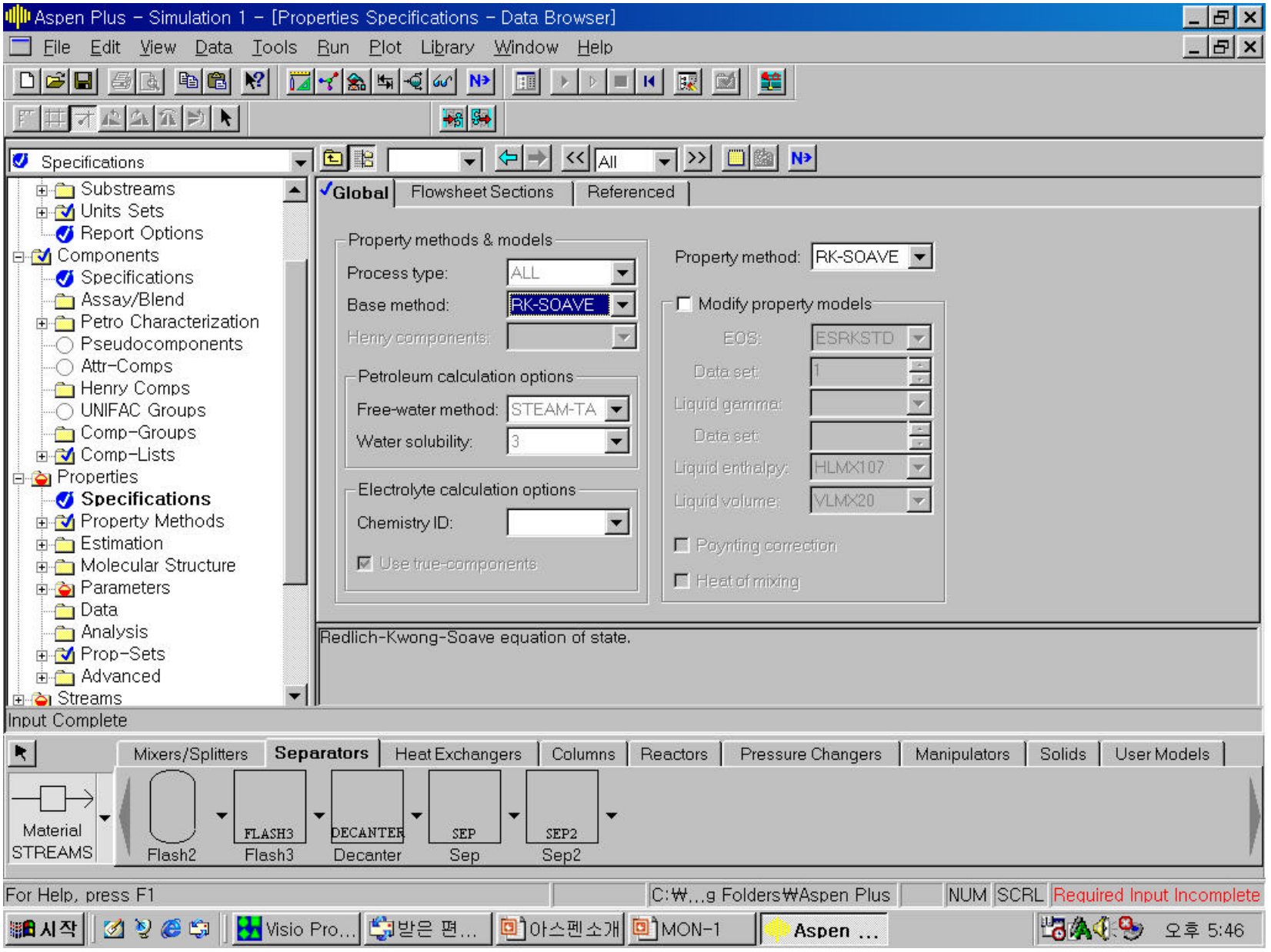
Dew P Calculation (General Process Information)



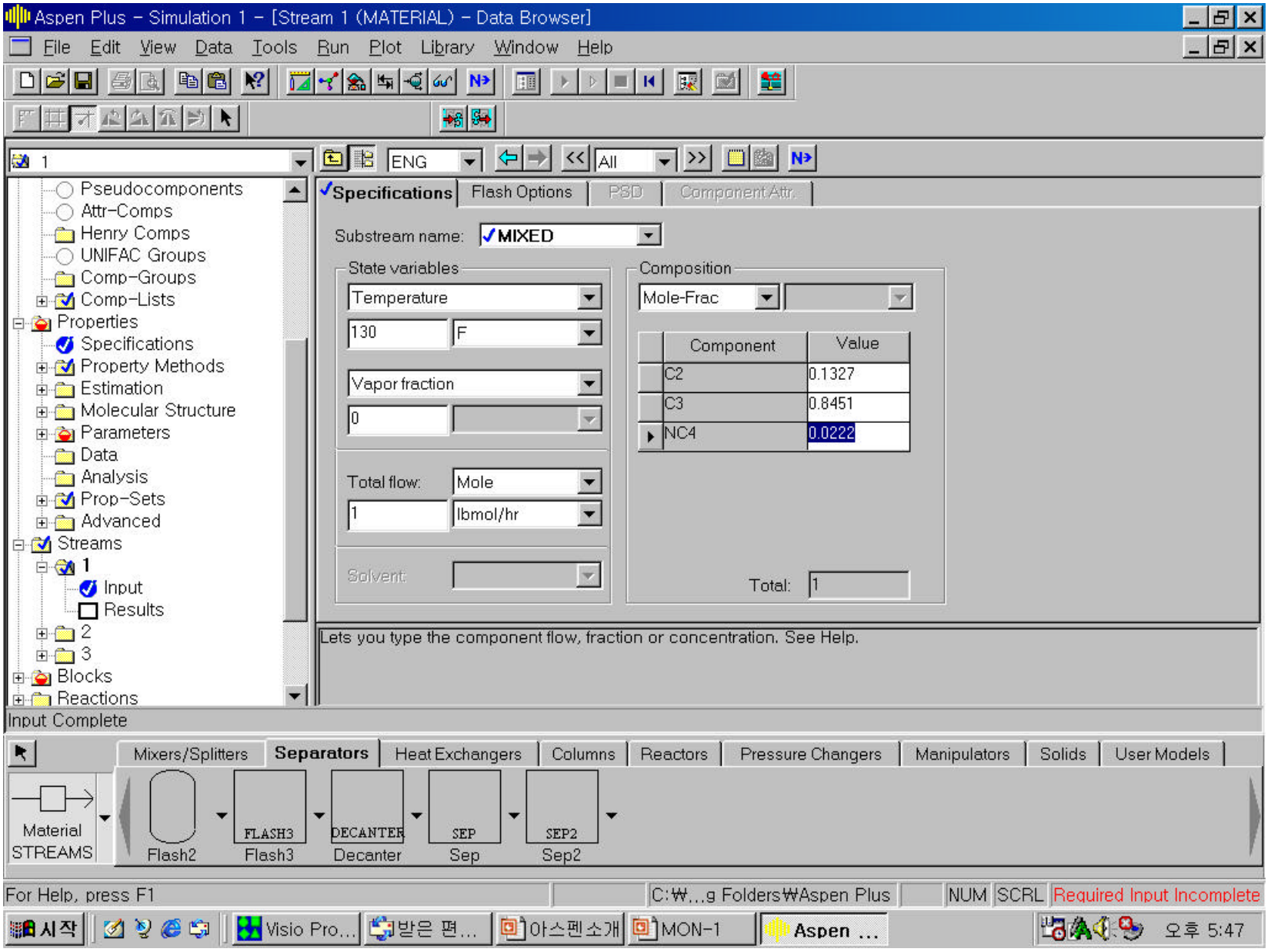
Dew P Calculation (Component Specification)



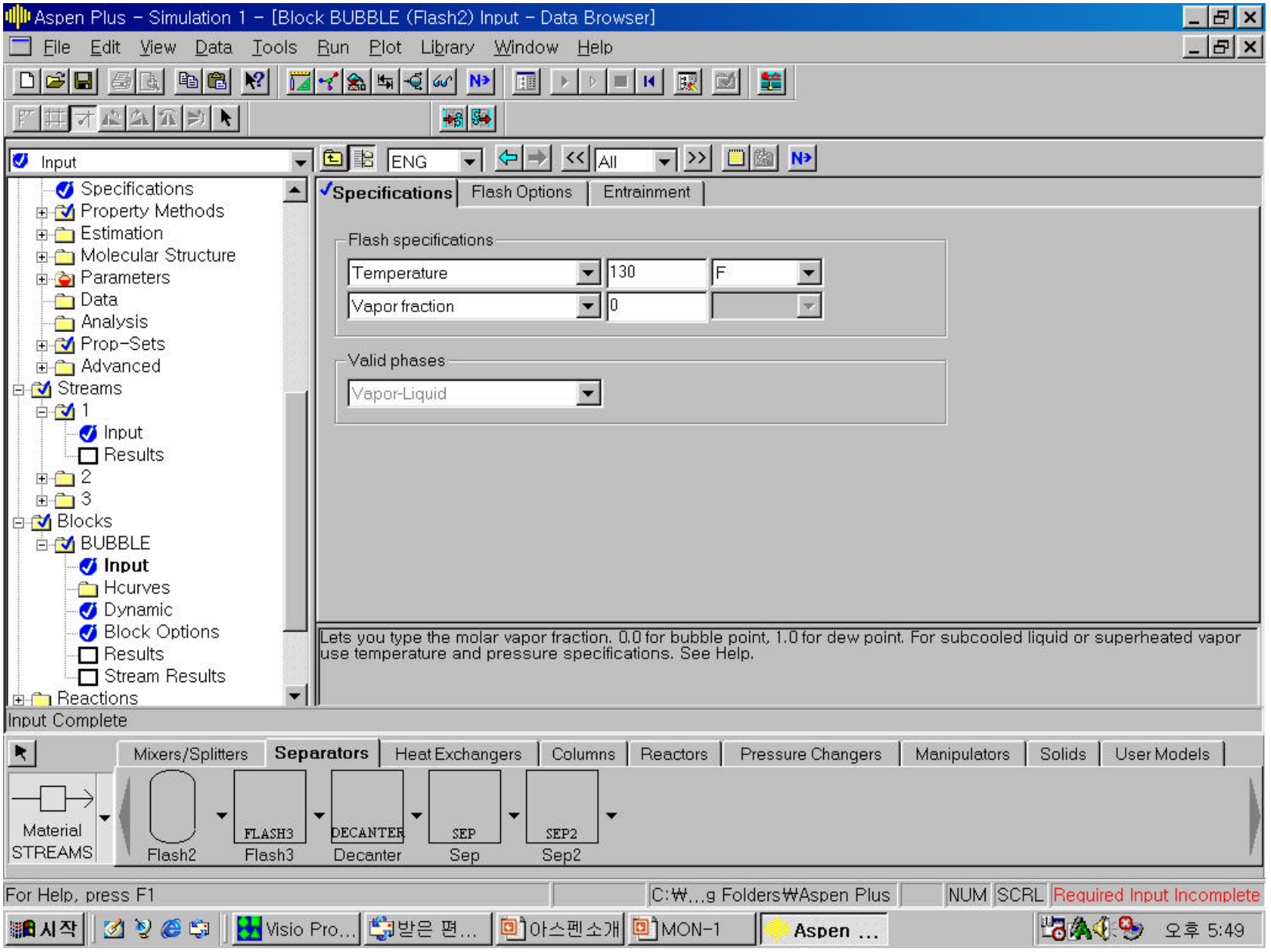
Dew P Calculation (Physical Property Specification)



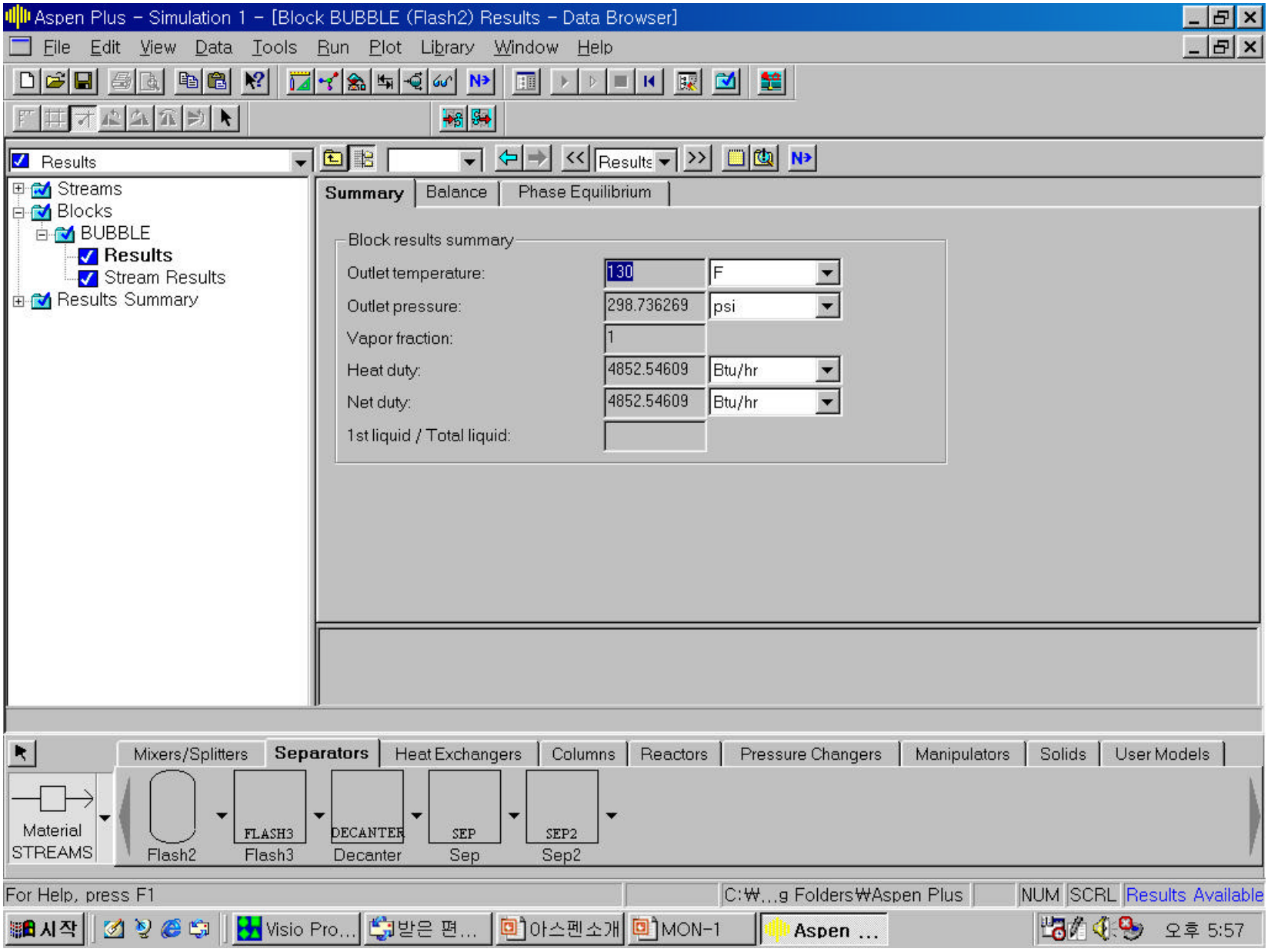
Dew P Calculation (Feed Stream Specification)



Dew P Calculation (Performance Specification)



Examine Results



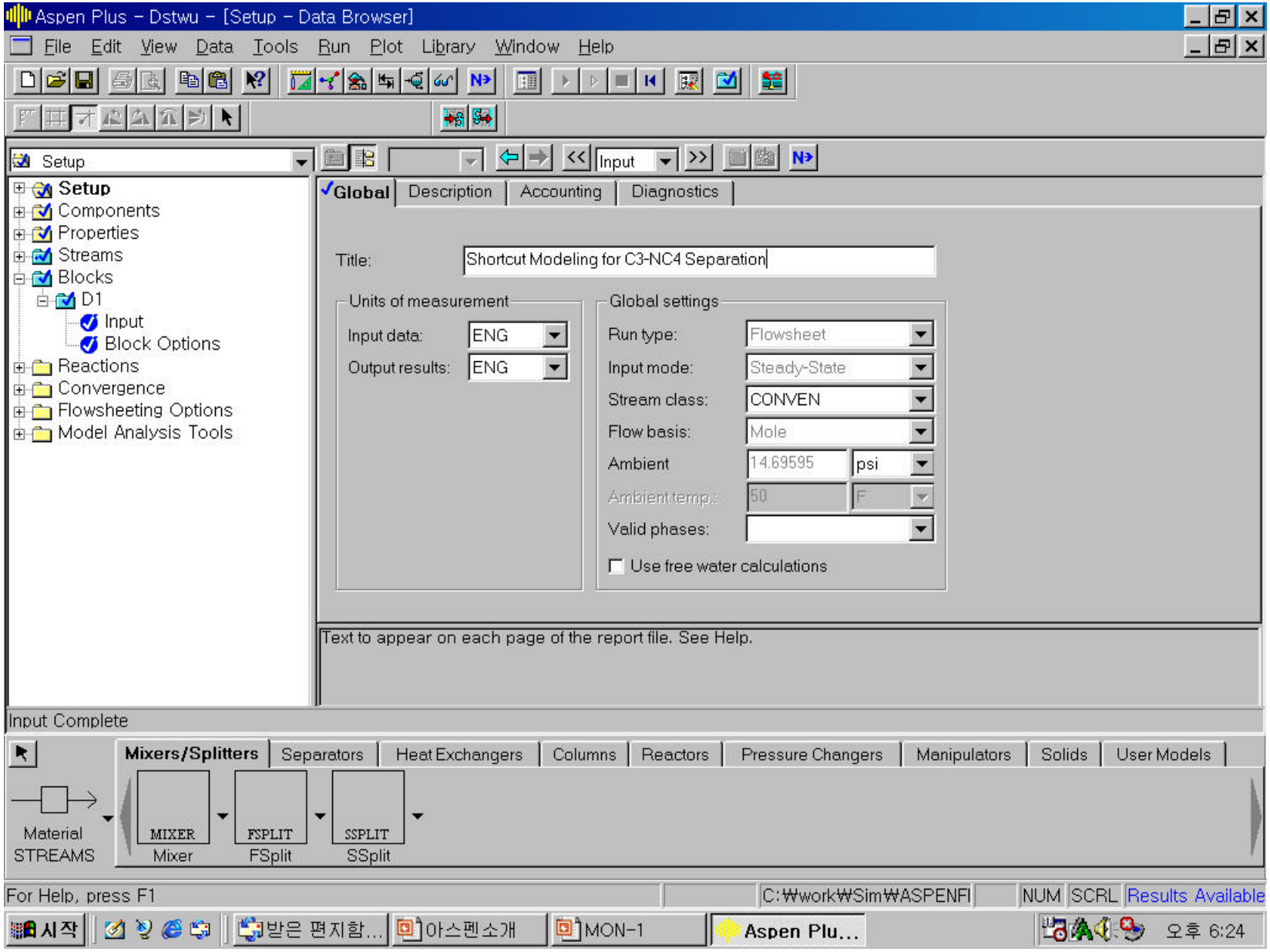
Dew Pressure Calculation Results

- Condenser type = partial condenser
- Condenser operating temperature = 130^{o}F
- Condenser Pressure = 299 psia
- Condenser pressure drop = 4 psia (assumed)
- Column pressure drop = 5 psia (assumed)

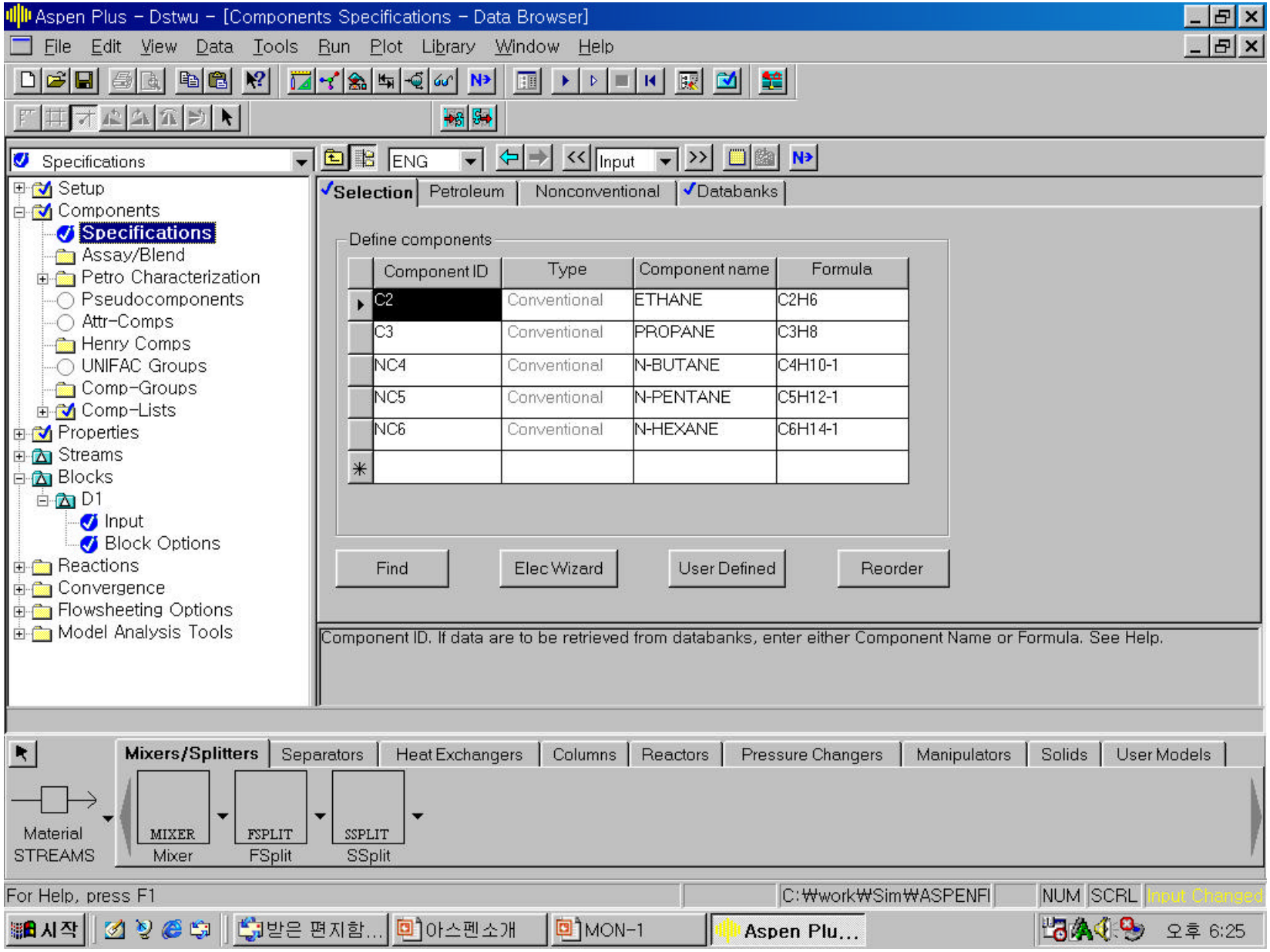
DSTWU modeling

- Partial condenser is utilized.
- RR = -1.75 (‘-’ means a multiple of minimum reflux ratio.)

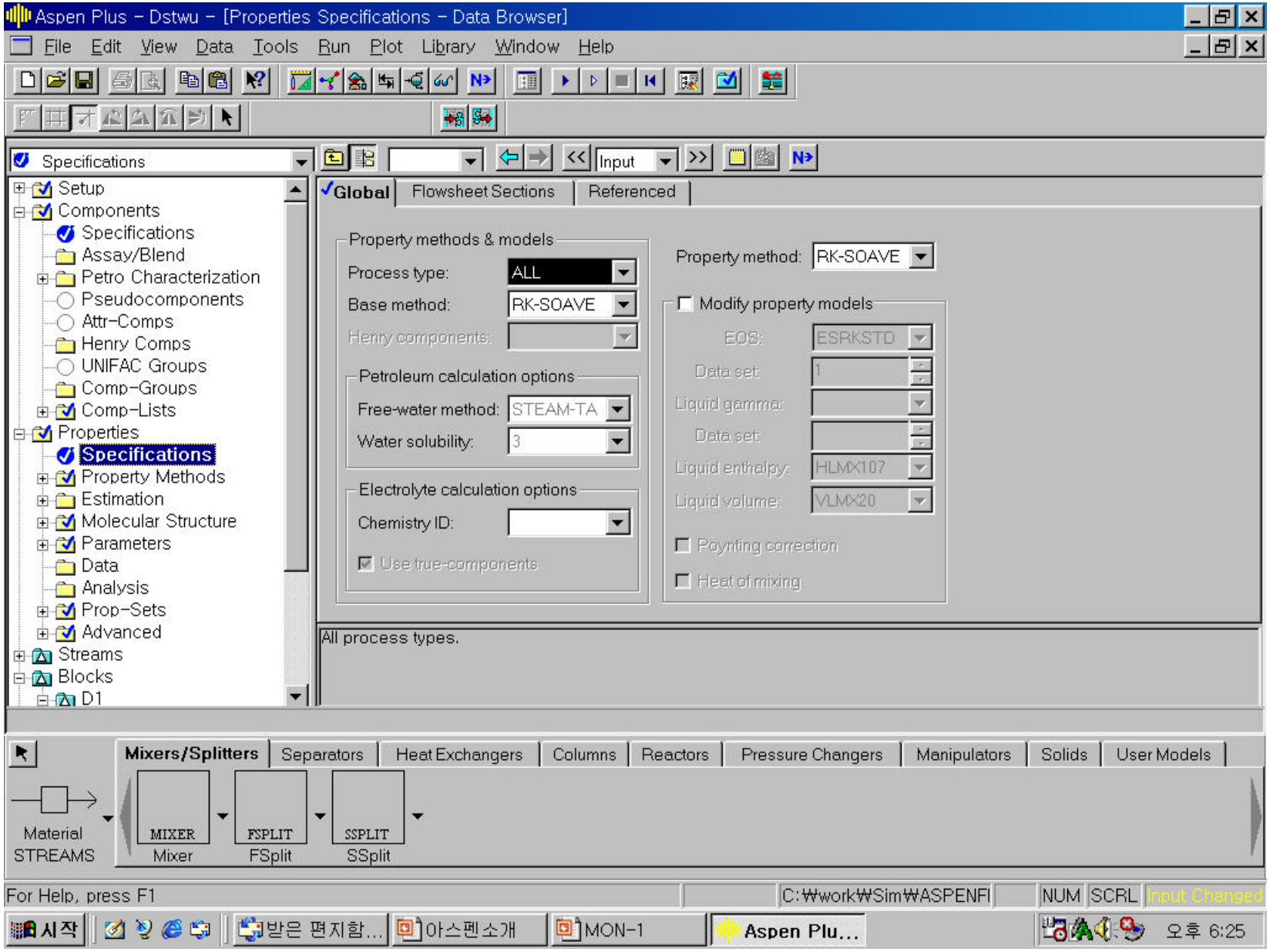
DSTWU modeling



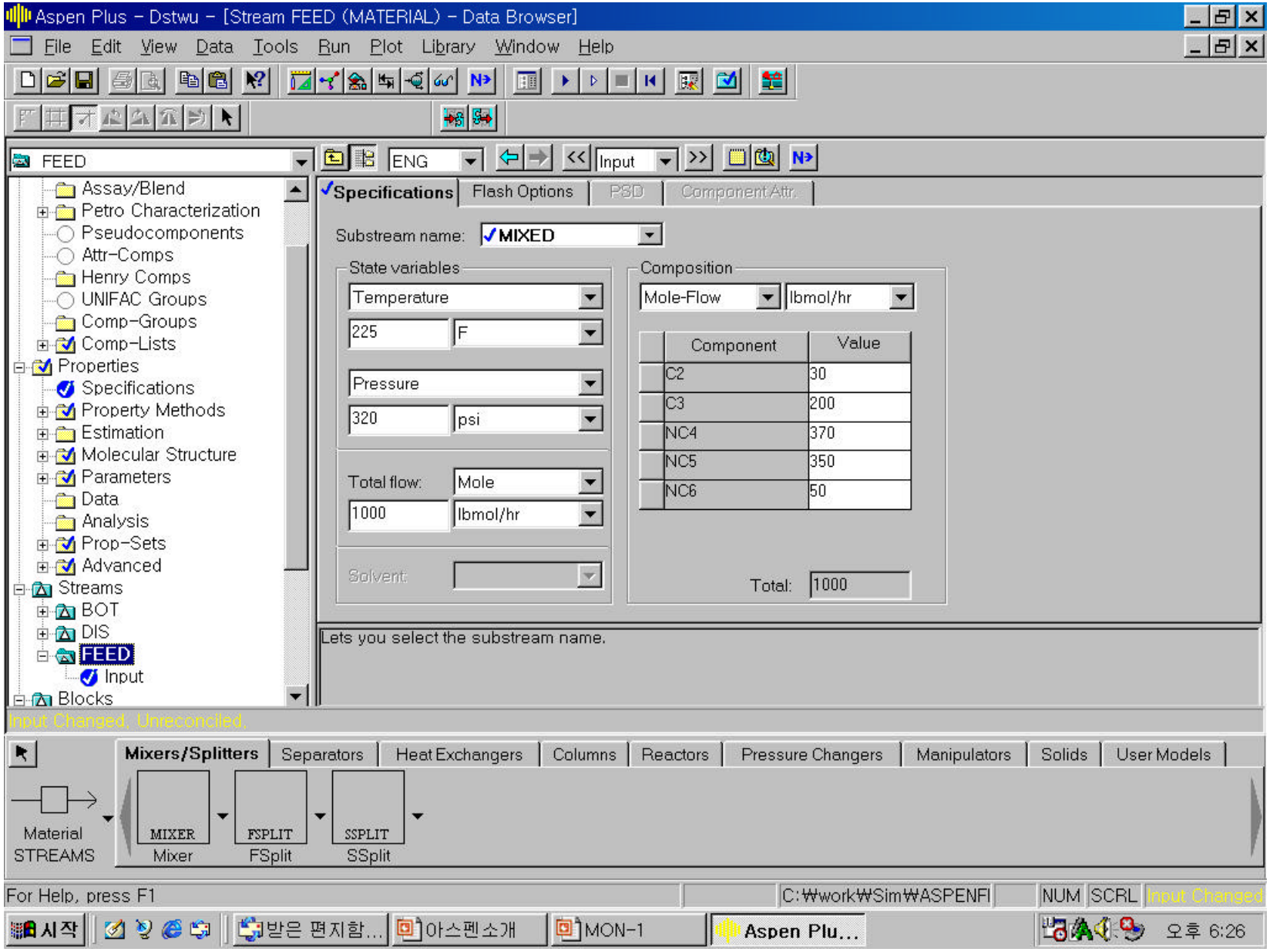
DSTWU modeling



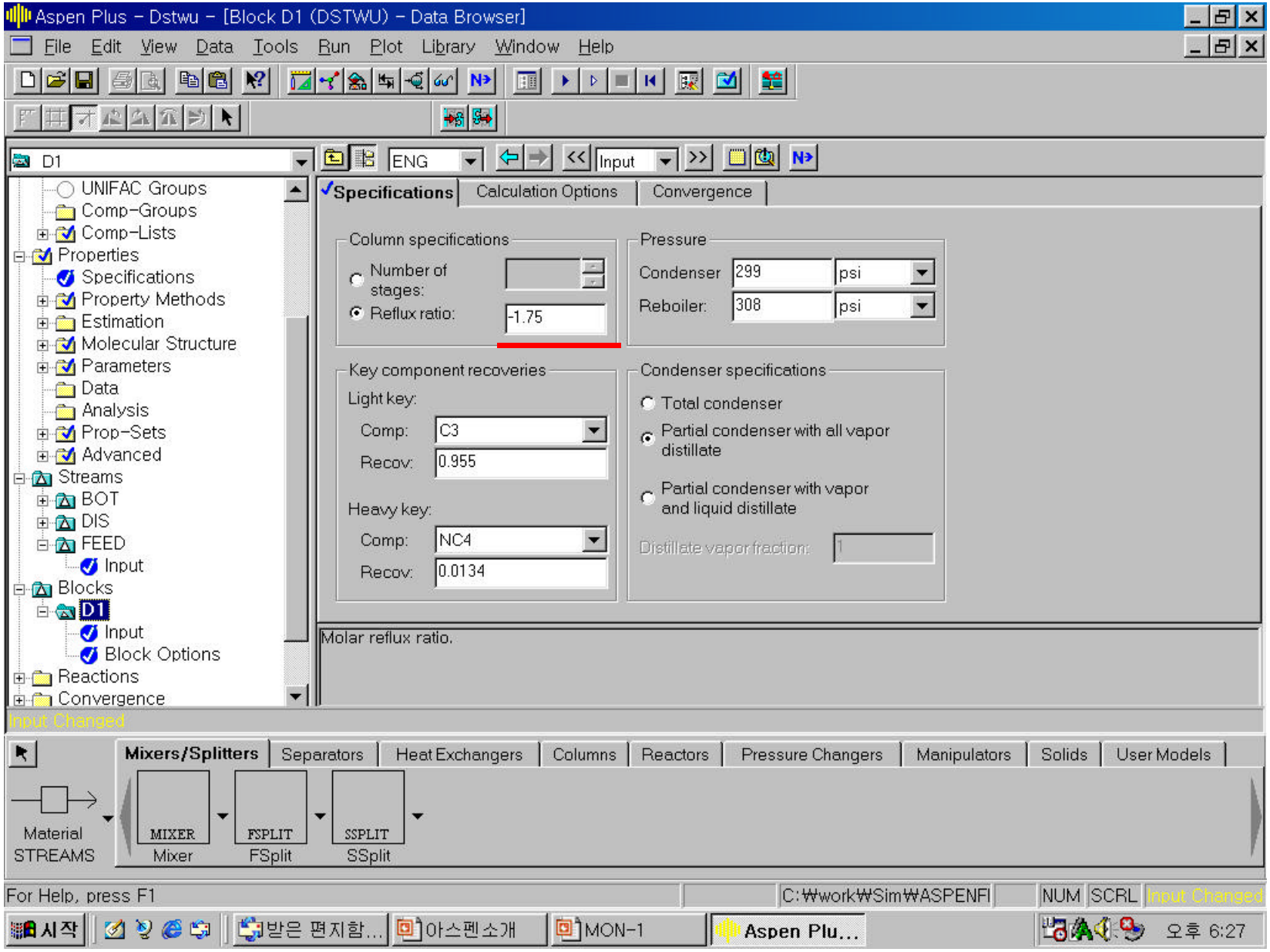
DSTWU modeling



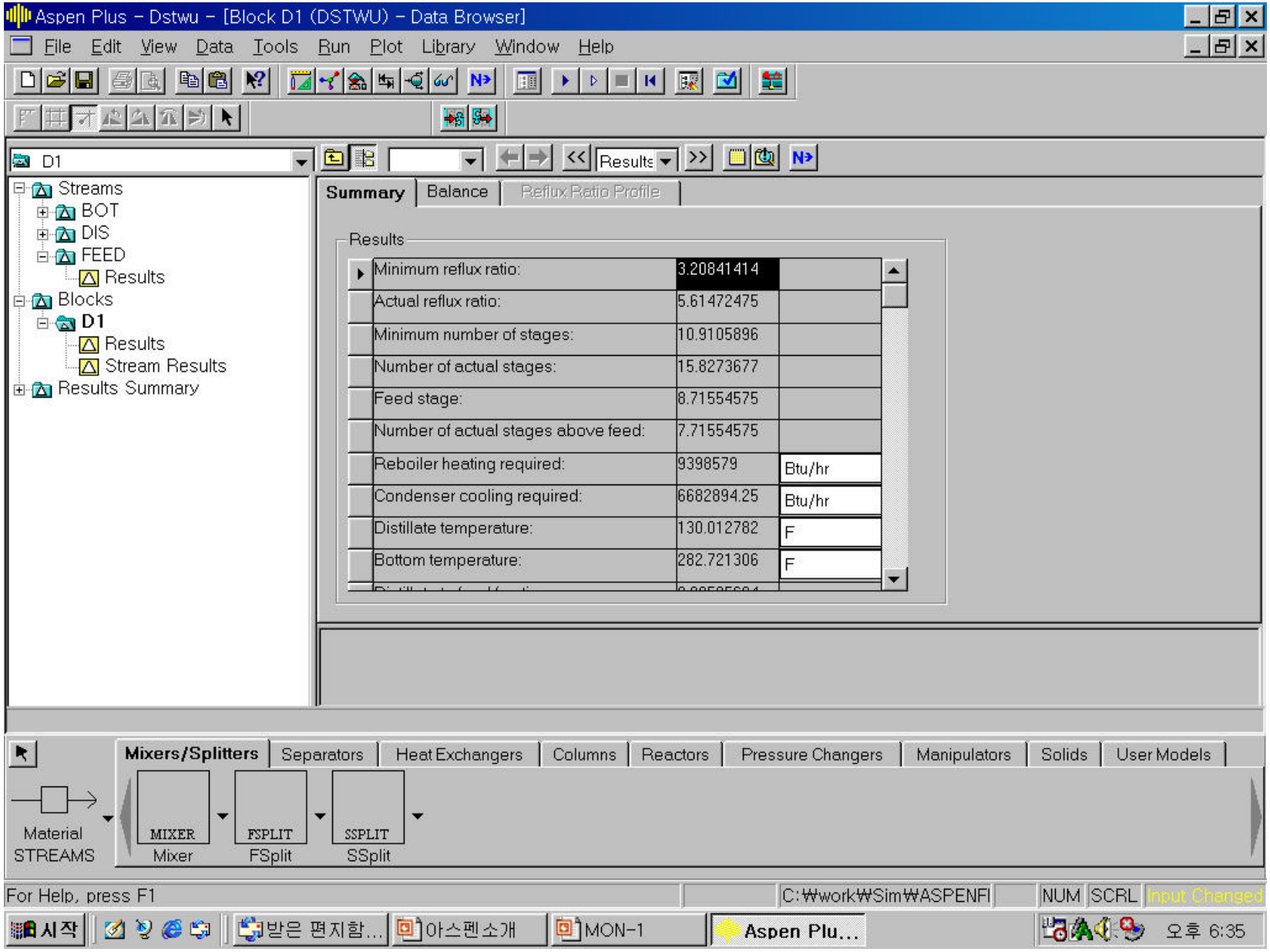
DSTWU modeling



DSTWU modeling



DSTWU modeling Results

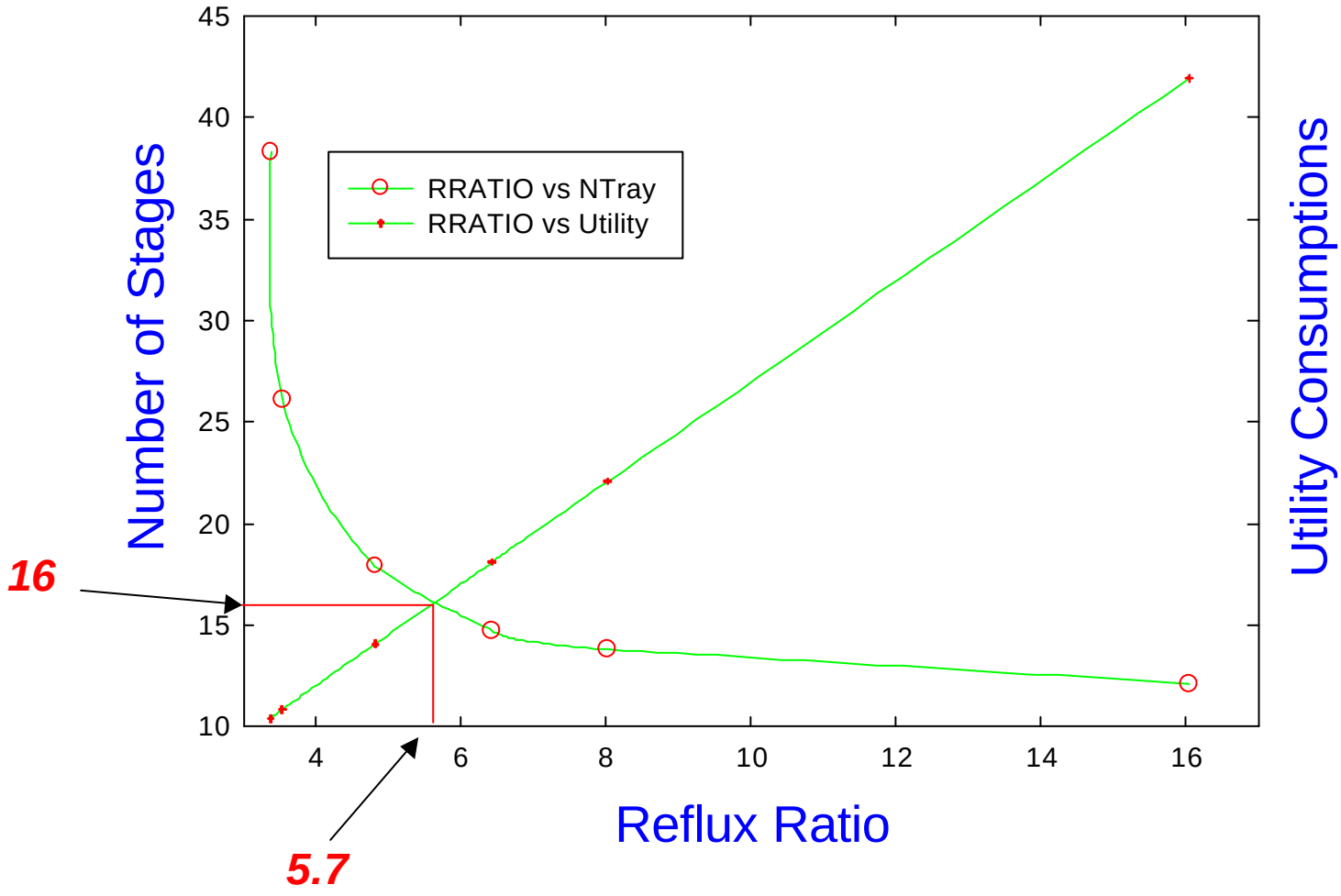


DSTWU modeling Case Study

R/R_{min}	Number of Tray	Reflux Ratio	Feed Tray	Condenser Duty	Reboiler Duty	Utility
1.00	**Infinitive**	**3.21**	-	-	-	-
1.05	38.3	3.37	19.7	3.82	6.54	10.36
1.10	26.1	3.53	13.7	4.06	6.77	10.83
1.50	17.9	4.81	9.7	5.67	8.39	14.06
2.00	14.7	6.42	8.0	7.69	10.40	18.09
2.50	13.8	8.02	7.7	9.67	12.39	22.06
5.00	12.1	16.04	6.9	19.60	22.32	41.92
Infinitive	**10.9**	**Infinitive**	-	-	-	-

- **Minimum Reflux Ratio = 3.21**
- **Minimum Number of Stages = 10.9**

Reflux Ratio vs. # of Stages & Utility Consumptions



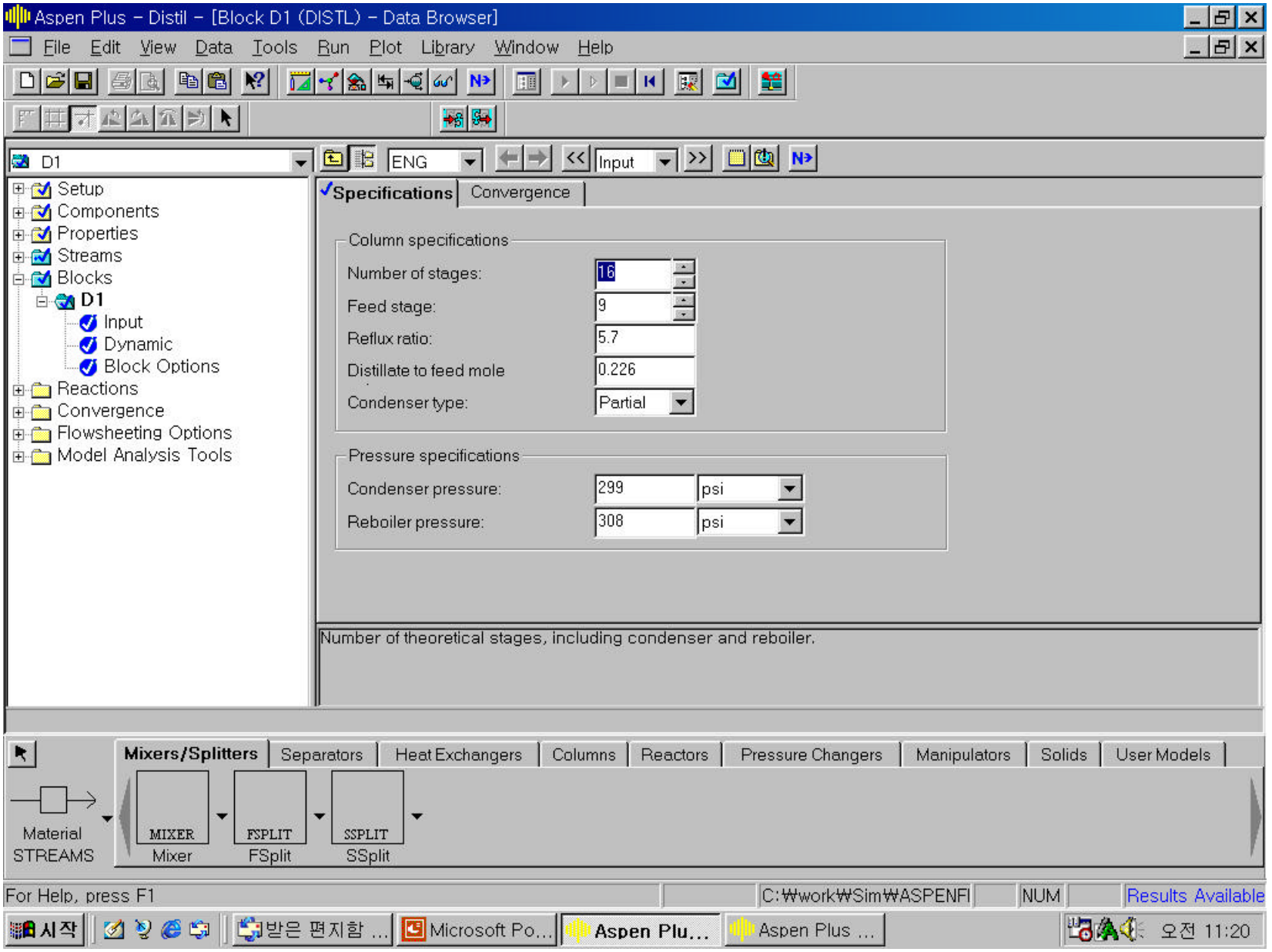
Shortcut Modeling Results using DSTWU

- File Name = DSTWU-F.bkp
- Optimum Reflux Ratio = 5.7
- Optimum Number of Stages = 16
- Feed Tray Location = 9
- Partial Condenser Temperature = 130 ^{o}F
- Overhead Condenser Heat Duty = 6.79 MM Btu/Hr
- Bottom Reboiler Heat Duty = 9.61 MM Btu/Hr
- C3 Recovery at Overhead Product = 95.5 %
- NC4 Recovery at Overhead Product = 1.34 %

Shortcut Modeling using DISTIL

- File Name = DISTIL.bkp
- Modeling using ‘ DISTIL’ is an intermediate step between DSTWU and RadFrac
- DSTWU :
  - N_{min}, R_{min},
  - Ratio, R/R_{min}
  - R_{opt}, N_{opt}, $FTRAY_{opt}$
- DISTIL tells us a preliminary modeling results such as condenser, reboiler heat duties, condenser temperature & material balances prior to performing rigorous modeling.

DISTIL (simulation flowshhet)



Comparison between ‘DSTWU’ and ‘DISTIL’

	DSTWU	DISTIL
Reflux Ratio	5.7	5.7
Number of Tray	16	16
Feed Tray Location	9	9
Condenser Temperature	130 ^{o}F	134 ^{o}F
Condenser Heat Duty	-6.79	-6.94
Reboiler Heat Duty	9.06	9.63
C3 Recovery at Top	95.5 %	93.0 %
NC4 Recovery at Top	1.34 %	2.7 %

RadFrac

- ***Objective:***

Discuss the minimum input required for the RadFrac fractionation model, and the use of design specifications and stage efficiencies

- ***Aspen Plus References:***

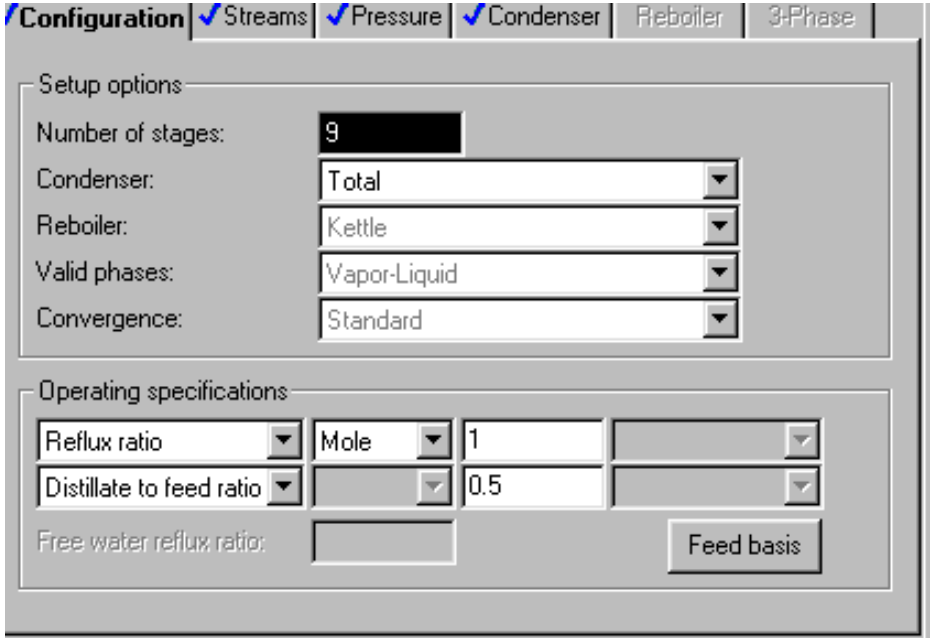
Unit Operation Models Reference Manual, Chapter 4, Columns

RadFrac: Rigorous Multistage Separation

- Vapor-Liquid or Vapor-Liquid-Liquid phase simulation of:
  - Ordinary distillation
  - Absorption, reboiled absorption
  - Stripping, reboiled stripping
  - Azeotropic distillation
  - Reactive distillation

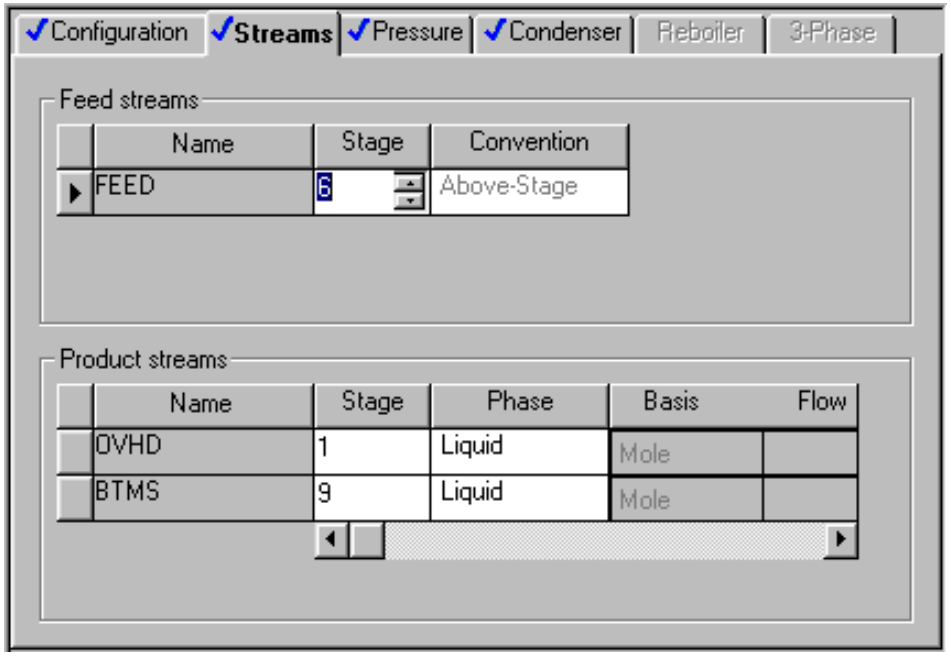
- Configuration options:
  - Any number of feeds
  - Any number of side draws
  - Total liquid draw off and pumparounds
  - Any number of heaters
  - Any number of decanters

RadFrac Setup Configuration Sheet



- Specify:
  - -Number of stages
  - -Condenser and reboiler configuration
  - -Two column operating specifications
  - -Valid phases
  - -Convergence

RadFrac Setup Streams Sheet



- Specify:
  - Feed stage location
  - Feed stream convention (see Help)

    ABOVE-STAGE:

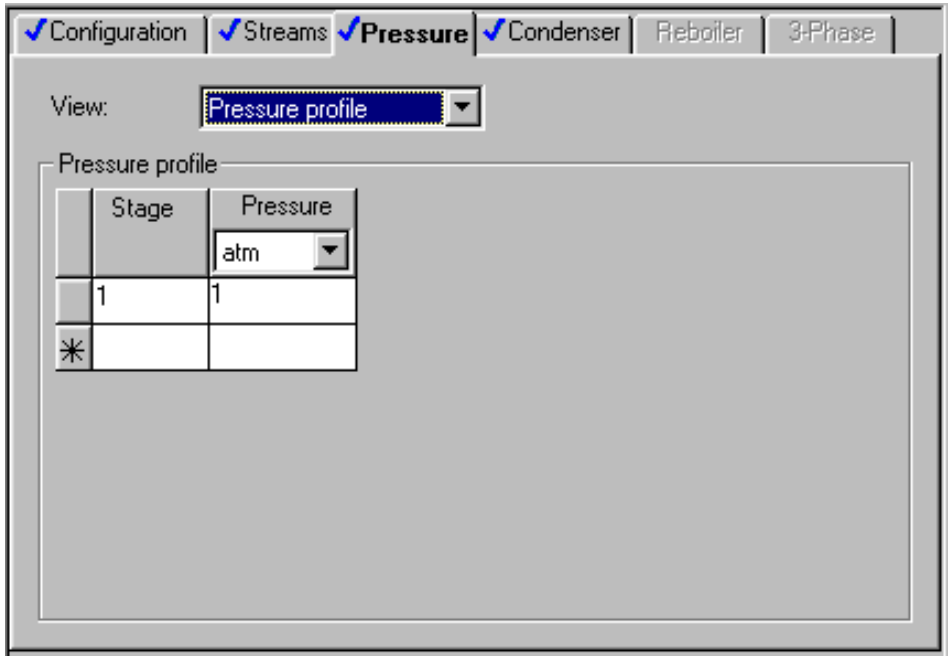
    Vapor from feed goes to stage above feed stage

    Liquid goes to feed stage

    ON-STAGE:

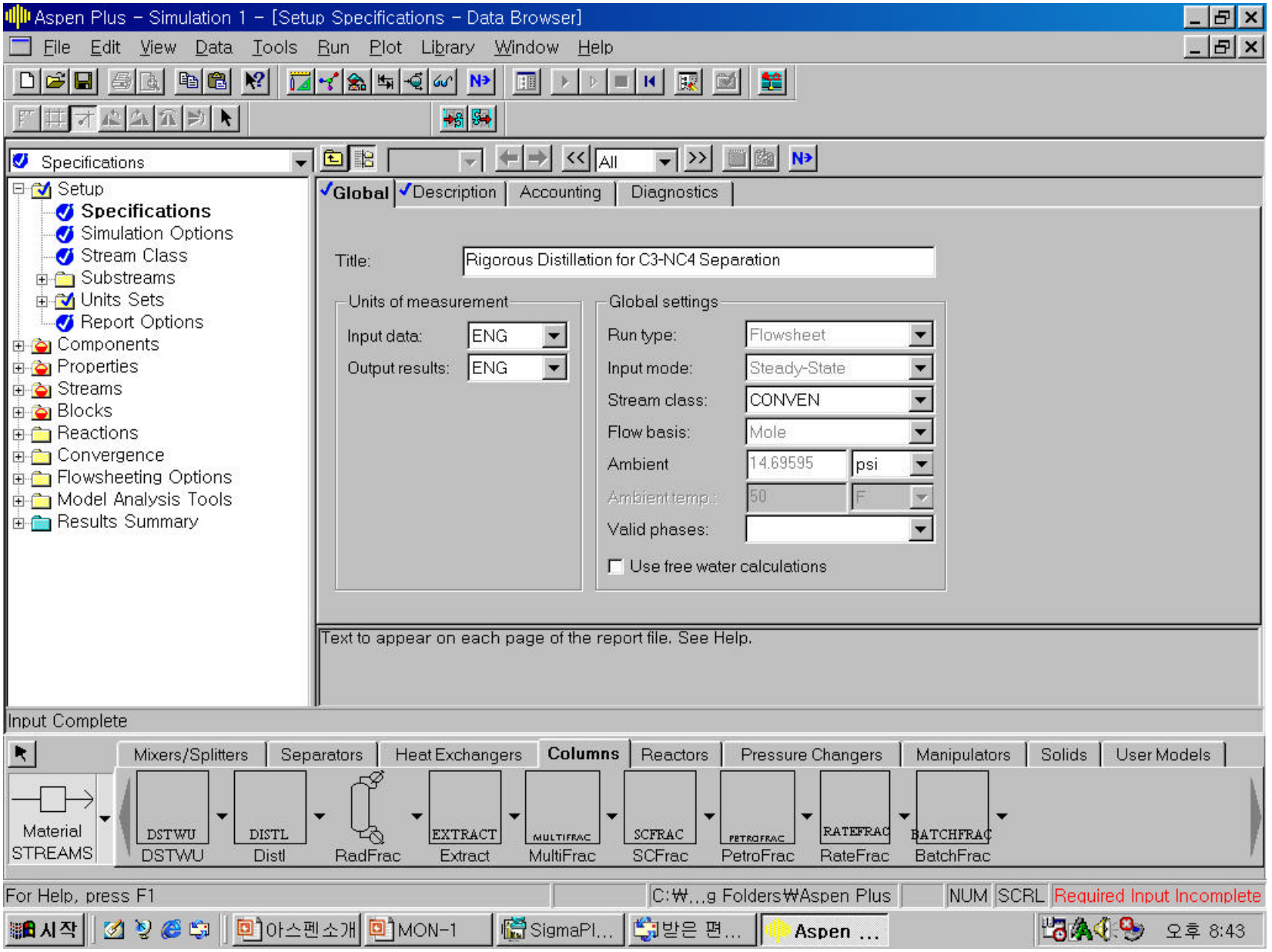
    Vapor & Liquid from feed go to specified feed stage

RadFrac Setup Pressure Sheet



- Specify one of:
  - Column pressure profile
  - Top/Bottom pressure
  - Section pressure drop

RadFrac


Aspen Plus – Simulation 1 – [Setup Specifications – Data Browser]
File Edit View Data Tools Run Plot Library Window Help
Specifications
All
Setup
Specifications
Simulation Options
Stream Class
Substreams
Units Sets
Report Options
Components
Properties
Streams
Blocks
Reactions
Convergence
Flowsheeting Options
Model Analysis Tools
Results Summary
Global
Description
Accounting
Diagnostics
Title:
Rigorous Distillation for C3-NC4 Separation
Units of measurement
Input data:
ENG
Output results:
ENG
Global settings
Run type:
Flowsheet
Input mode:
Steady-State
Stream class:
CONVEN
Flow basis:
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Ambient
14.69595
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Ambient temp.:
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Valid phases:
Use free water calculations
Text to appear on each page of the report file. See Help.
Input Complete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material
STREAMS
DSTWU
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EXTRACT
Extract
MULTIFRAC
MultiFrac
SCFRAC
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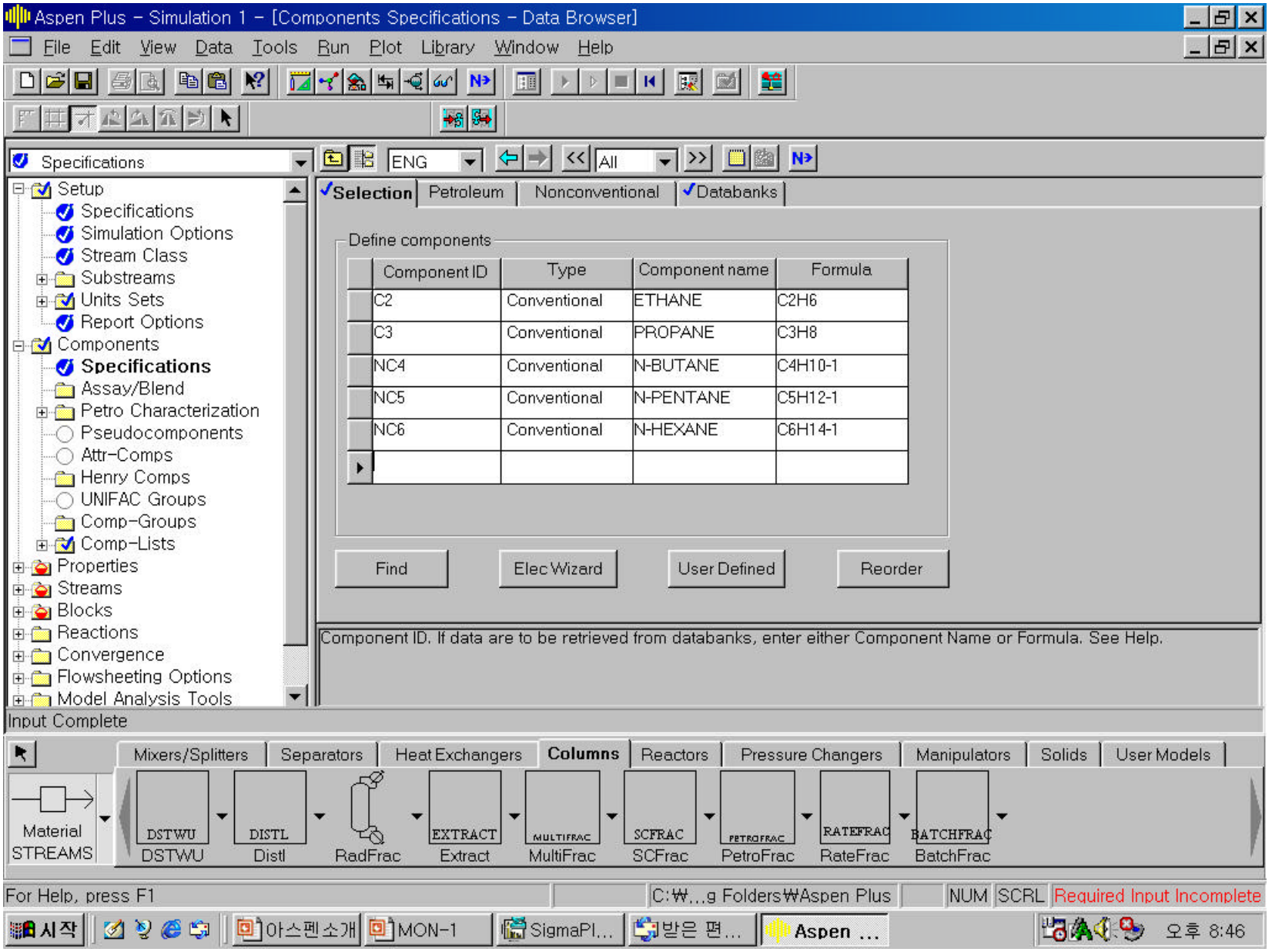
RadFrac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File Edit View Data Tools Run Plot Library Window Help
Specifications
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Simulation Options
Stream Class
Substreams
Units Sets
Report Options
Components
Specifications
Assay/Blend
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Properties
Streams
Blocks
Reactions
Convergence
Flowsheeting Options
Model Analysis Tools
Selection
Petroleum
Nonconventional
Databanks
Define components
Component ID
Type
Component name
Formula
C2
Conventional
ETHANE
C2H6
C3
Conventional
PROPANE
C3H8
NC4
Conventional
N-BUTANE
C4H10-1
NC5
Conventional
N-PENTANE
C5H12-1
NC6
Conventional
N-HEXANE
C6H14-1
Find
Elec Wizard
User Defined
Reorder
Component ID. If data are to be retrieved from databanks, enter either Component Name or Formula. See Help.
Input Complete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
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RateFrac
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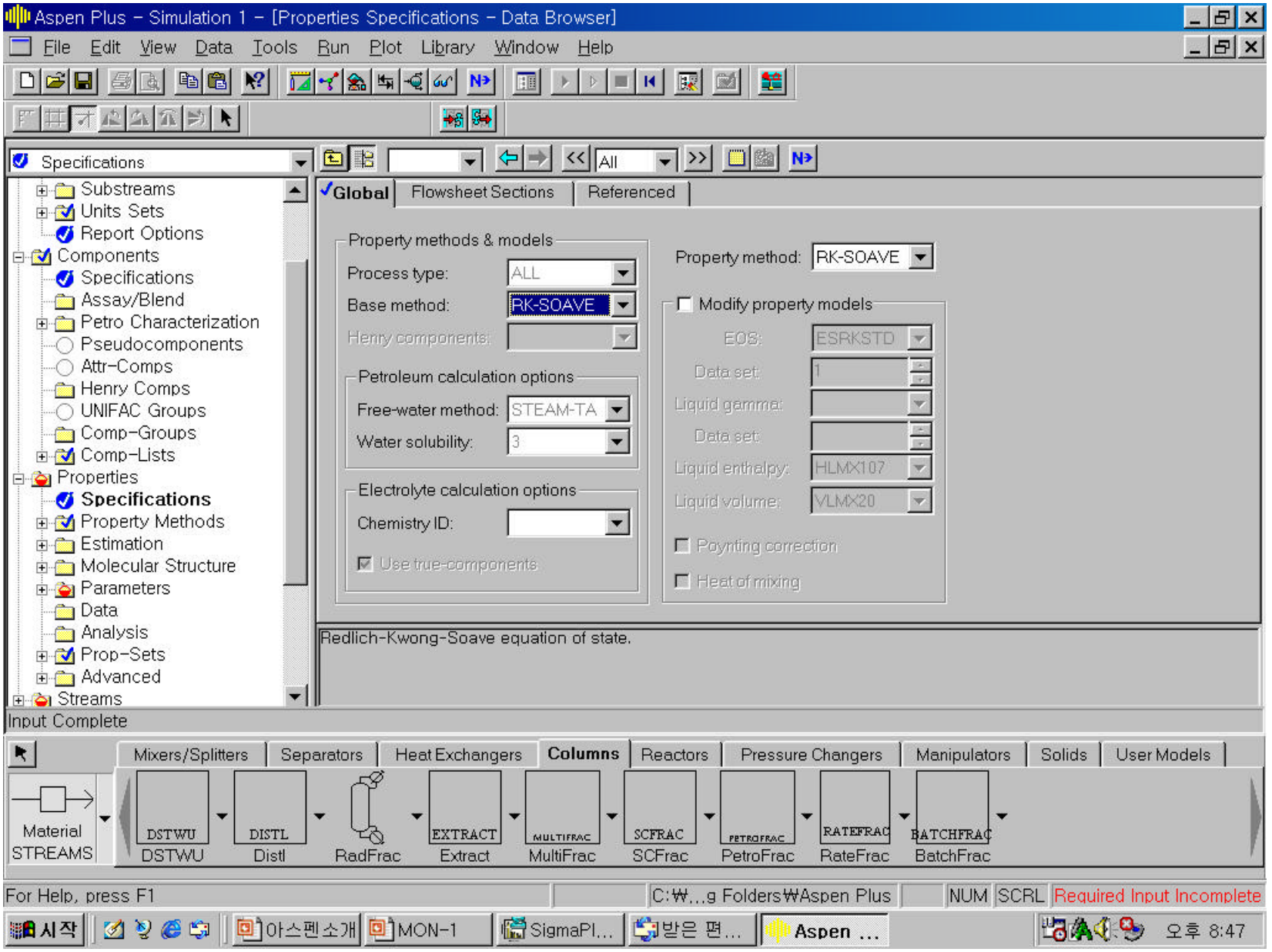
RadFrac


Aspen Plus – Simulation 1 – [Properties Specifications – Data Browser]
File Edit View Data Tools Run Plot Library Window Help
Specifications
All
Substreams
Units Sets
Report Options
Components
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Assay/Blend
Petro Characterization
Pseudocomponents
Attr-Comps
Henry Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Data
Analysis
Prop-Sets
Advanced
Streams
Global
Flowsheet Sections
Referenced
Property methods & models
Process type: ALL
Base method: RK-SOAVE
Henry components:
Petroleum calculation options
Free-water method: STEAM-TA
Water solubility: 3
Electrolyte calculation options
Chemistry ID:
Use true-components
Property method: RK-SOAVE
Modify property models
EOS: ESRKSTD
Data set: 1
Liquid gamma:
Data set:
Liquid enthalpy: HLMX107
Liquid volume: VLMX20
Poynting correction
Heat of mixing
Redlich-Kwong-Soave equation of state.
Input Complete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material STREAMS
DSTWU DSTWU
DISTL Distl
RadFrac
EXTRACT Extract
MULTIFRAC MultiFrac
SCFRAC SCFrac
PETROFRAC PetroFrac
RATEFRAC RateFrac
BATCHFRAC BatchFrac
For Help, press F1
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받은 편...
Aspen ...
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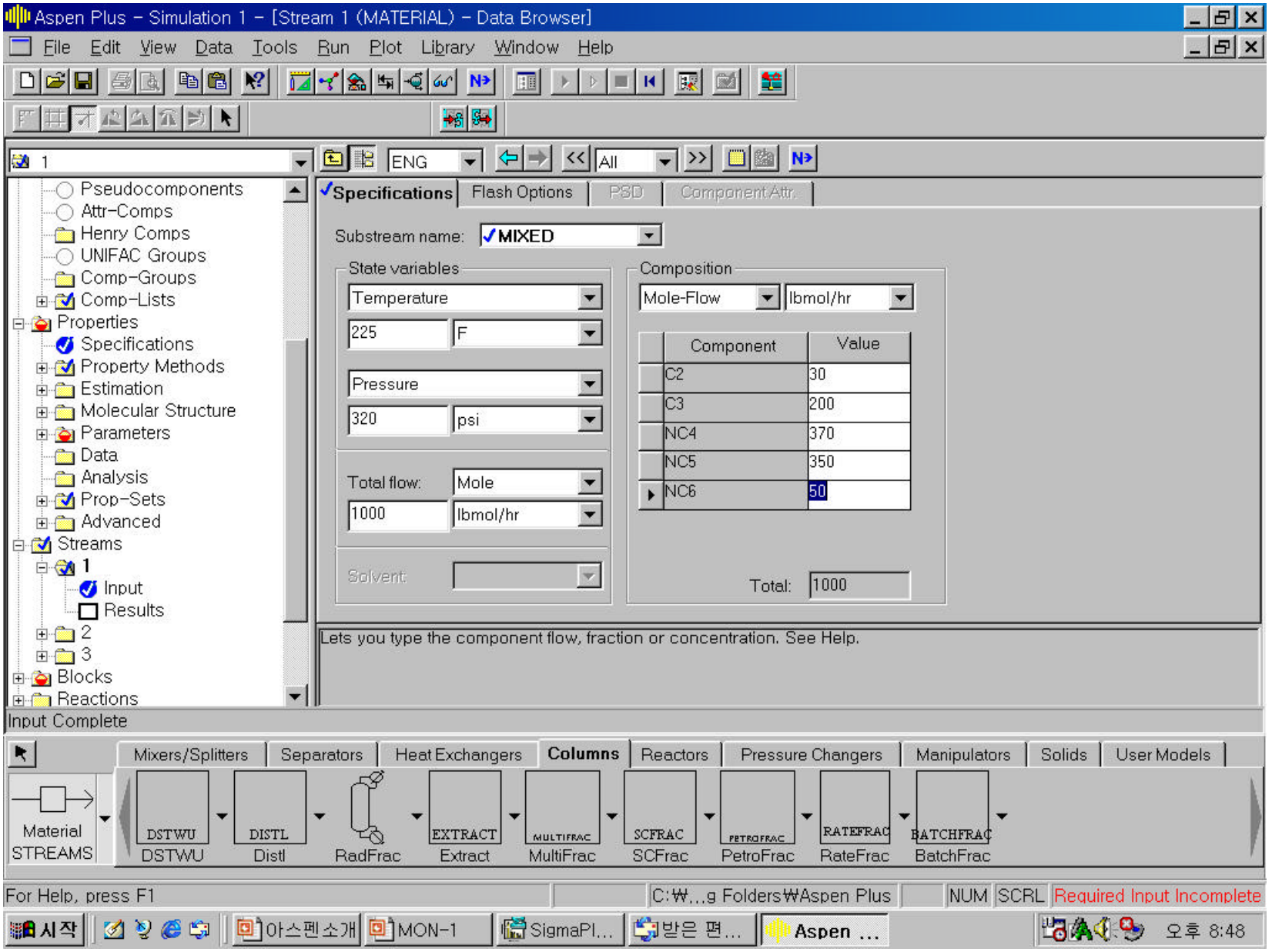
RadFrac


Aspen Plus - Simulation 1 - [Stream 1 (MATERIAL) - Data Browser]
File Edit View Data Tools Run Plot Library Window Help
Pseudocomponents
Attr-Comps
Henry Comps
UNIFAC Groups
Comp-Groups
Comp-Lists
Properties
Specifications
Property Methods
Estimation
Molecular Structure
Parameters
Data
Analysis
Prop-Sets
Advanced
Streams
1
Input
Results
2
3
Blocks
Reactions
Specifications
Flash Options
PSD
Component Attr.
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State variables
Temperature
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F
Pressure
320
psi
Total flow:
Mole
1000
lbmol/hr
Solvent:
Composition
Mole-Flow
lbmol/hr
Component
Value
C2
30
C3
200
NC4
370
NC5
350
NC6
50
Total:
1000
Lets you type the component flow, fraction or concentration. See Help.
Input Complete
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material STREAMS
DSTWU
Distl
RadFrac
Extract
MultiFrac
SCFrac
PetroFrac
RateFrac
BatchFrac
For Help, press F1
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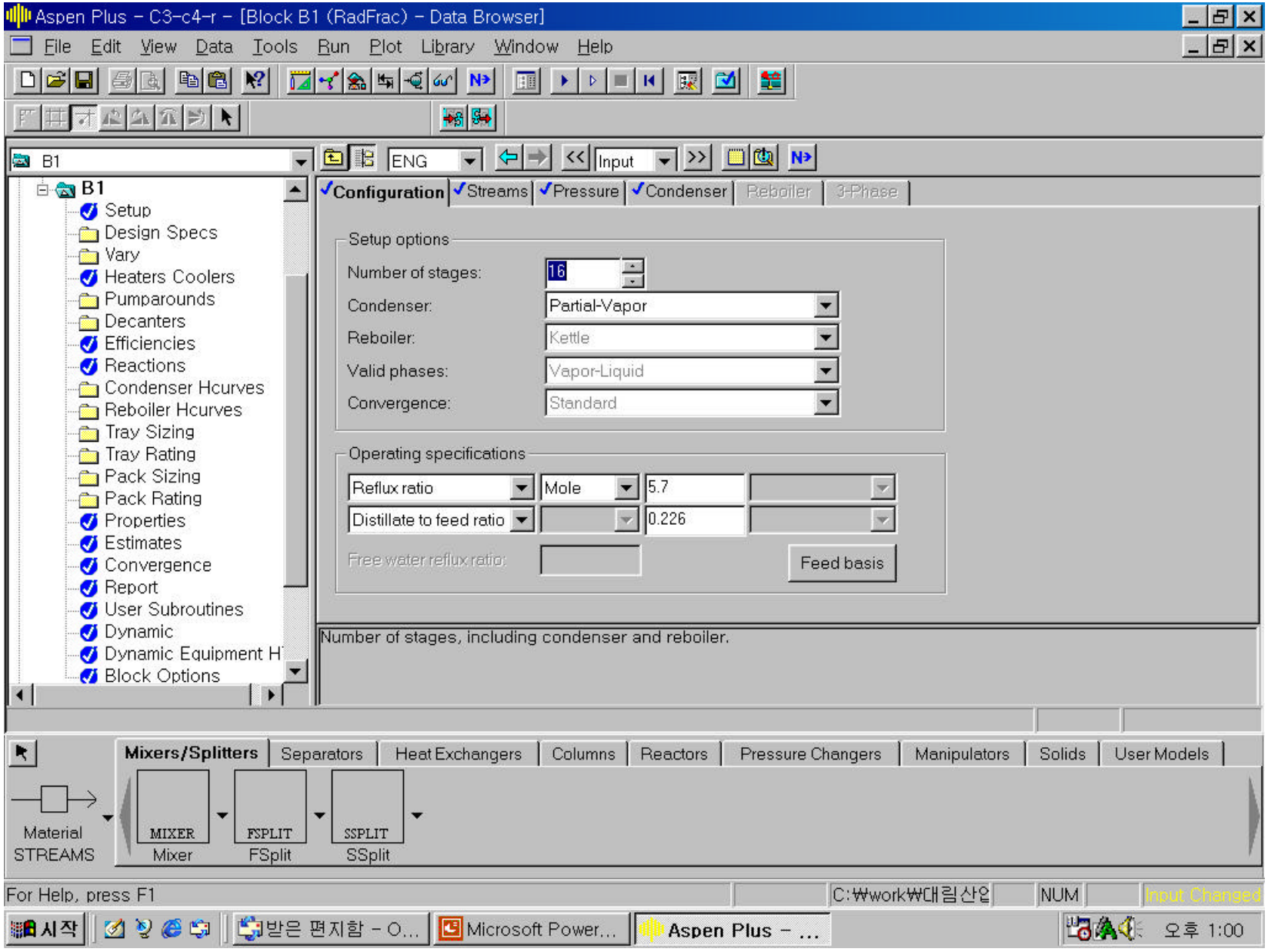
RadFrac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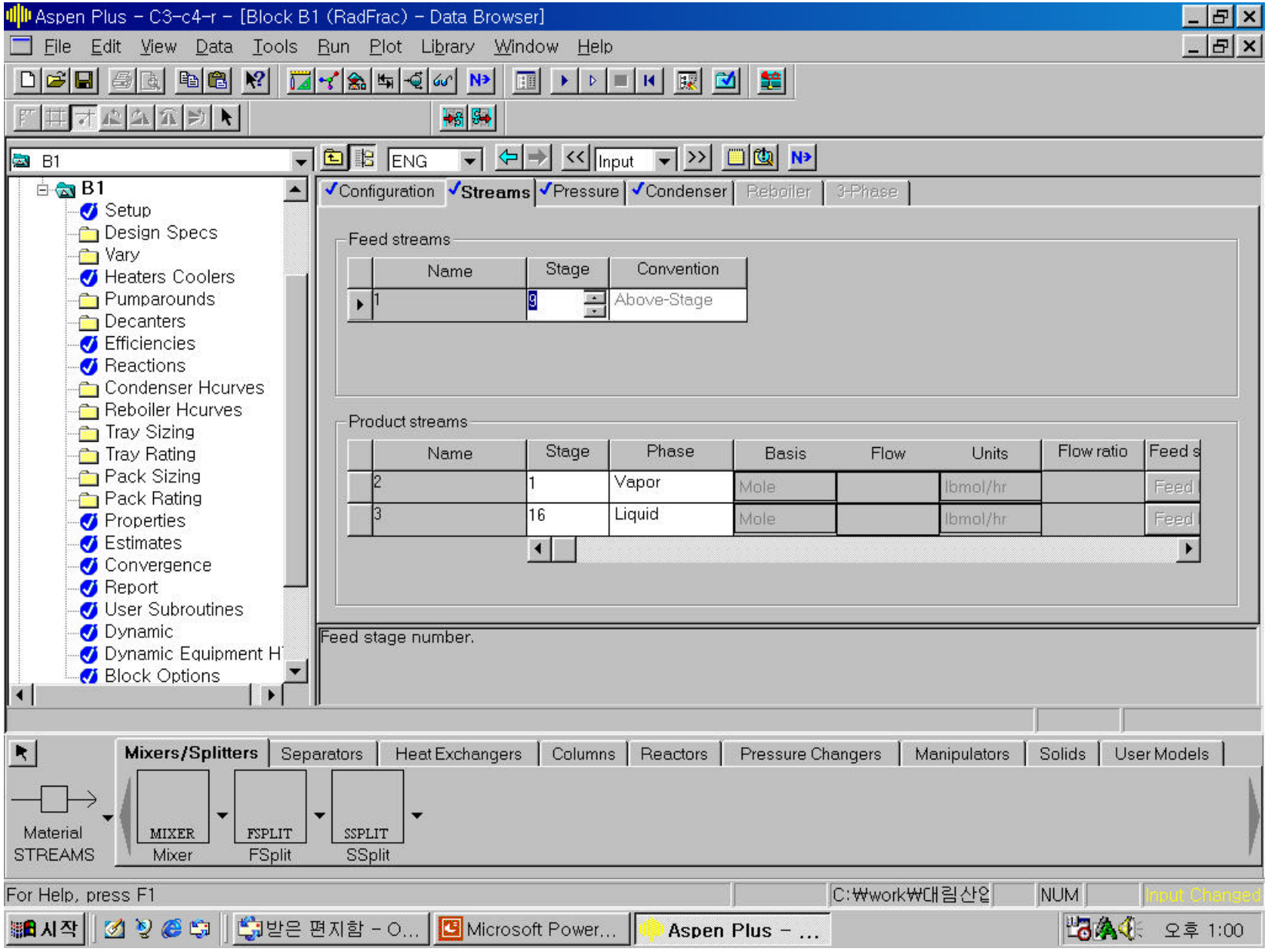
File Edit View Data Tools Run Plot Library Window Help
B1
ENG
Input
B1
Setup
Design Specs
Vary
Heaters Coolers
Pumparounds
Decanters
Efficiencies
Reactions
Condenser Hcurves
Reboiler Hcurves
Tray Sizing
Tray Rating
Pack Sizing
Pack Rating
Properties
Estimates
Convergence
Report
User Subroutines
Dynamic
Dynamic Equipment H
Block Options
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
Setup options
Number of stages:
16
Condenser:
Partial-Vapor
Reboiler:
Kettle
Valid phases:
Vapor-Liquid
Convergence:
Standard
Operating specifications
Reflux ratio
Mole
5.7
Distillate to feed ratio
0.226
Free water reflux ratio:
Feed basis
Number of stages, including condenser and reboiler.
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material
STREAMS
MIXER
Mixer
FSPLIT
FSplit
SSPLIT
SSplit
For Help, press F1
C:₩work₩대림산업
NUM
Input Changed
시작
받은 편지함 - O...
Microsoft Power...
Aspen Plus – ...
오후 1:00

RadFrac


Aspen Plus – C3-c4-r – [Block B1 (RadFrac) – Data Browser]
File Edit View Data Tools Run Plot Library Window Help
B1
ENG
Input
B1
Setup
Design Specs
Vary
Heaters Coolers
Pumparounds
Decanters
Efficiencies
Reactions
Condenser Hcurves
Reboiler Hcurves
Tray Sizing
Tray Rating
Pack Sizing
Pack Rating
Properties
Estimates
Convergence
Report
User Subroutines
Dynamic
Dynamic Equipment H
Block Options
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
Feed streams
Name
Stage
Convention
1
9
Above-Stage
Product streams
Name
Stage
Phase
Basis
Flow
Units
Flow ratio
Feed s
2
1
Vapor
Mole
lbmol/hr
Feed
3
16
Liquid
Mole
lbmol/hr
Feed
Feed stage number.
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material
STREAMS
MIXER
Mixer
FSPLIT
FSplit
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SSplit
For Help, press F1
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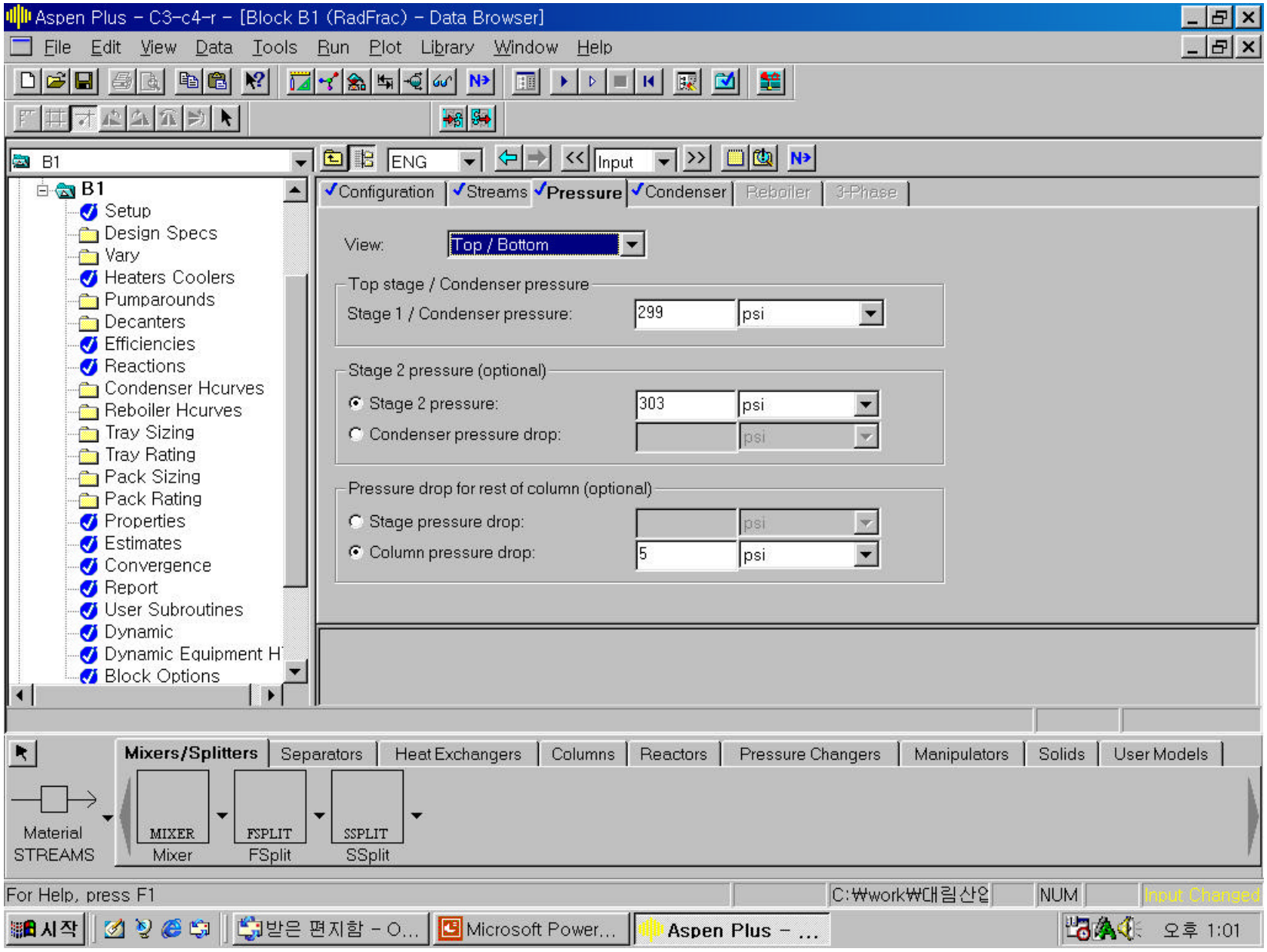
NUM
Input Changed
시작
받은 편지함 - O...
Microsoft Power...
Aspen Plus – ...
오후 1:00

RadFrac


Aspen Plus – C3-c4-r – [Block B1 (RadFrac) – Data Browser]
File Edit View Data Tools Run Plot Library Window Help
B1
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Setup
Design Specs
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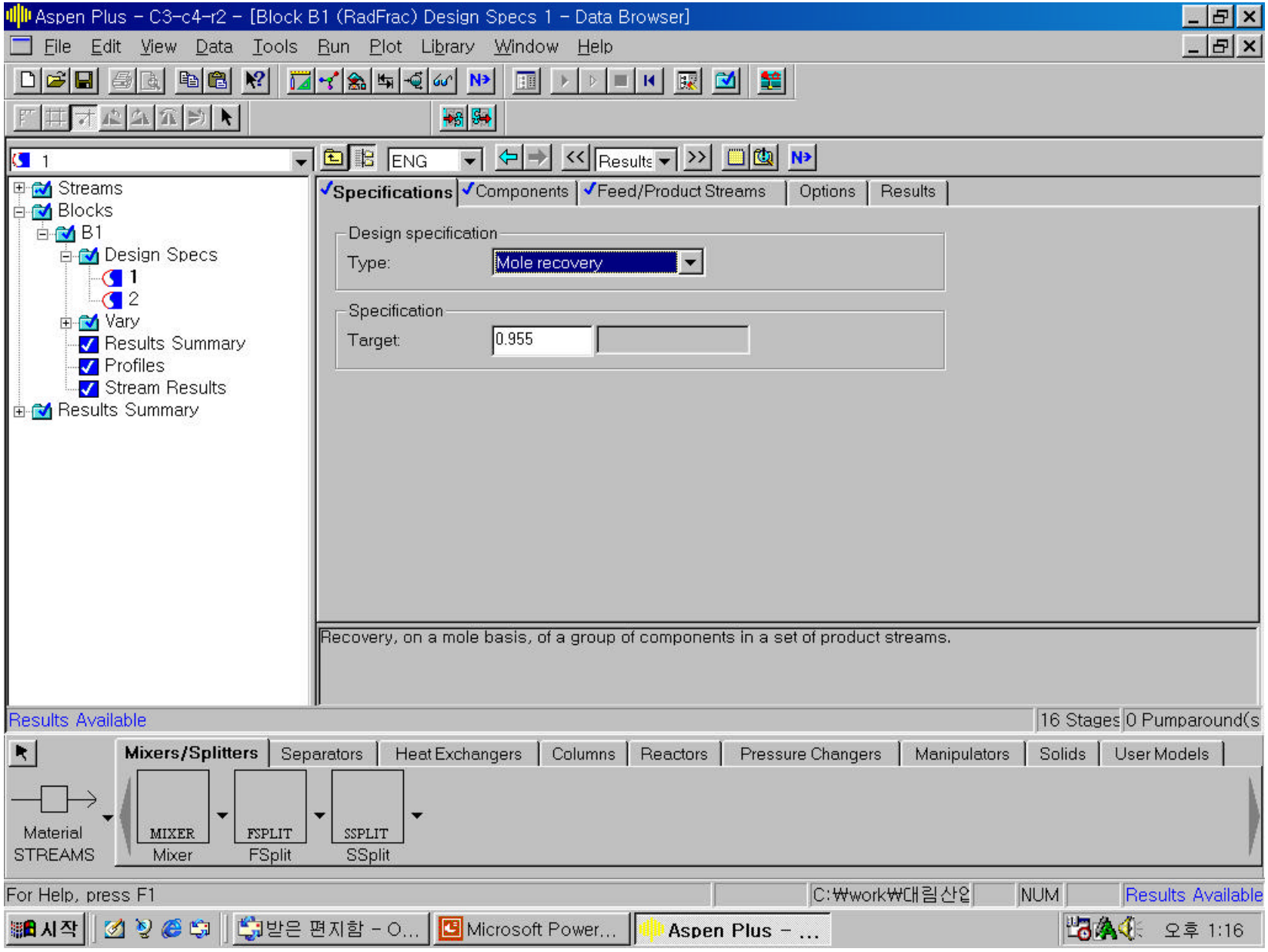
Reboiler Hcurves
Tray Sizing
Tray Rating
Pack Sizing
Pack Rating
Properties
Estimates
Convergence
Report
User Subroutines
Dynamic
Dynamic Equipment H
Block Options
Configuration
Streams
Pressure
Condenser
Reboiler
3-Phase
View:
Top / Bottom
Top stage / Condenser pressure
Stage 1 / Condenser pressure:
299
psi
Stage 2 pressure (optional)
Stage 2 pressure:
303
psi
Condenser pressure drop:
psi
Pressure drop for rest of column (optional)
Stage pressure drop:
psi
Column pressure drop:
5
psi
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
Material
STREAMS
MIXER
Mixer
FSPLIT
FSplit
SSPLIT
SSplit
For Help, press F1
C:₩work₩대림산업
NUM
Input Changed
시작
받은 편지함 - O...
Microsoft Power...
Aspen Plus - ...
오후 1:01

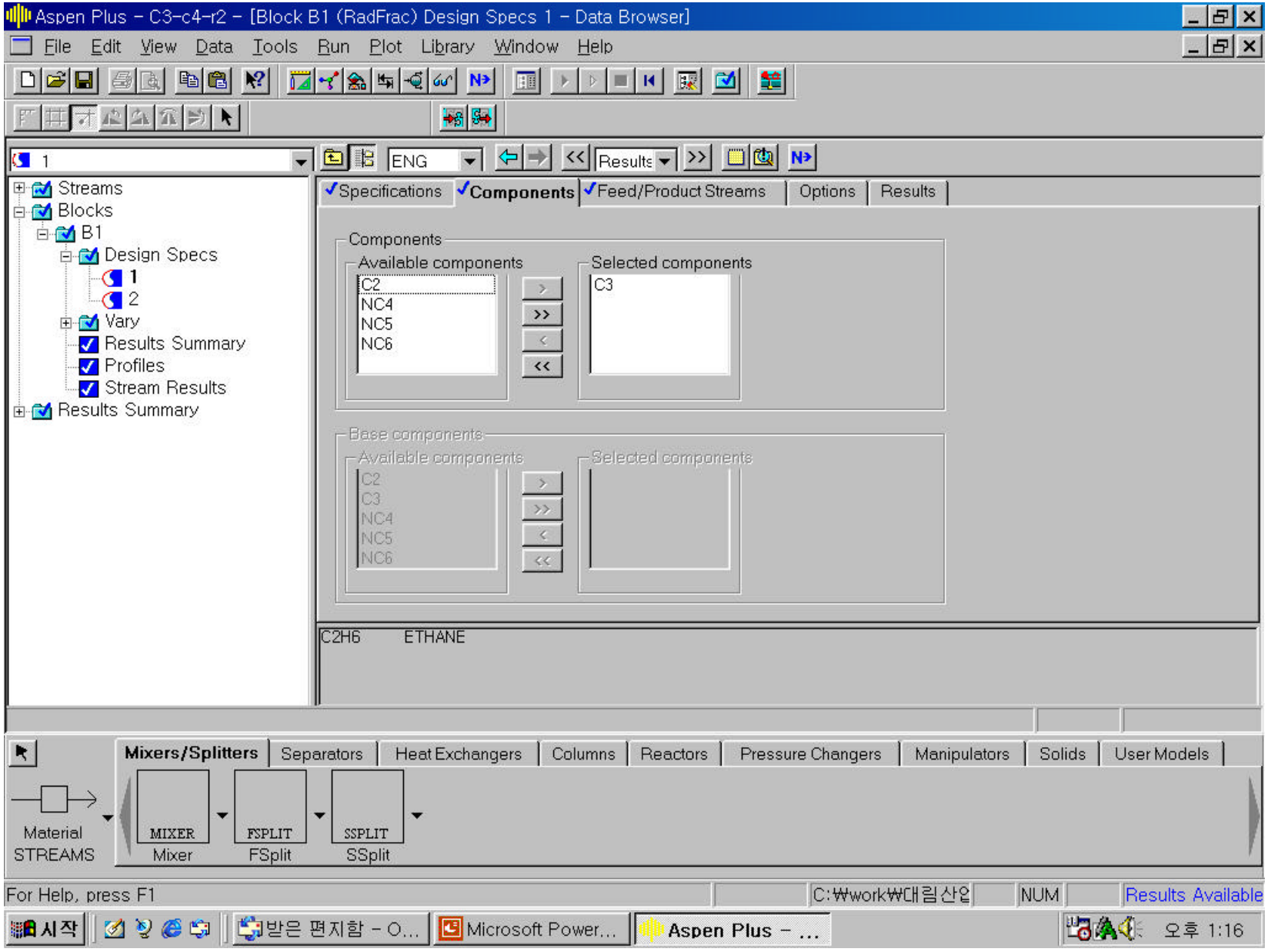
Comparison between ‘DSTWU’, ‘DISTIL’, and ‘RadFrac1’

	DSTWU	DISTIL	RadFrac1
Reflux Ratio	5.7	5.7	5.7
Number of Tray	16	16	16
Feed Tray Location	9	9	9
Condenser Temperature	130 ^{o}F	134 ^{o}F	135.3 ^{o}F
Condenser Heat Duty	-6.79	-6.94	-7.11
Reboiler Heat Duty	9.06	9.63	9.79
C3 Recovery at Top	95.5 %	93.0 %	92.0 %
NC4 Recovery at Top	1.34 %	2.7 %	3.22 %

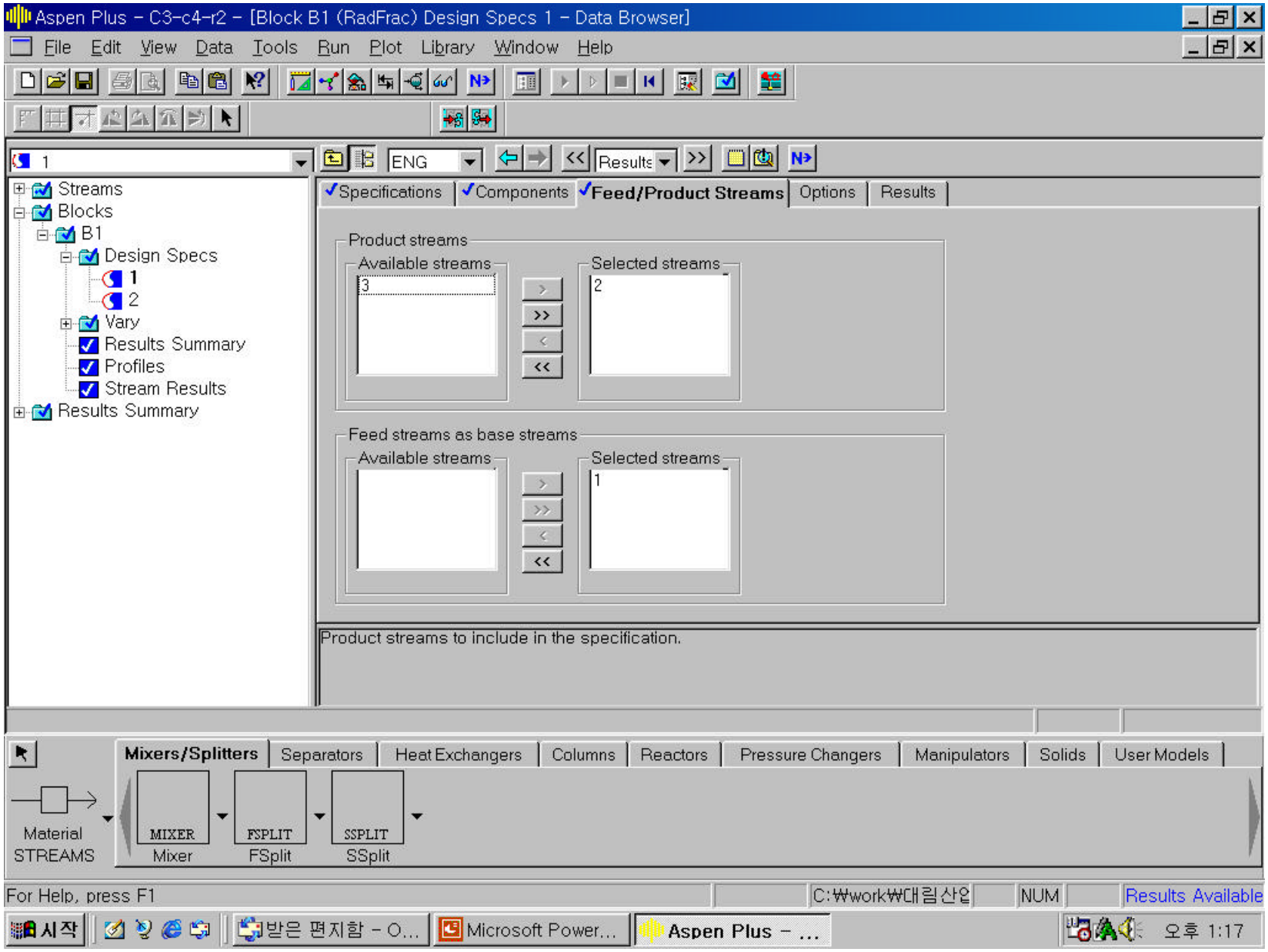
RadFrac (Design Spec 1)



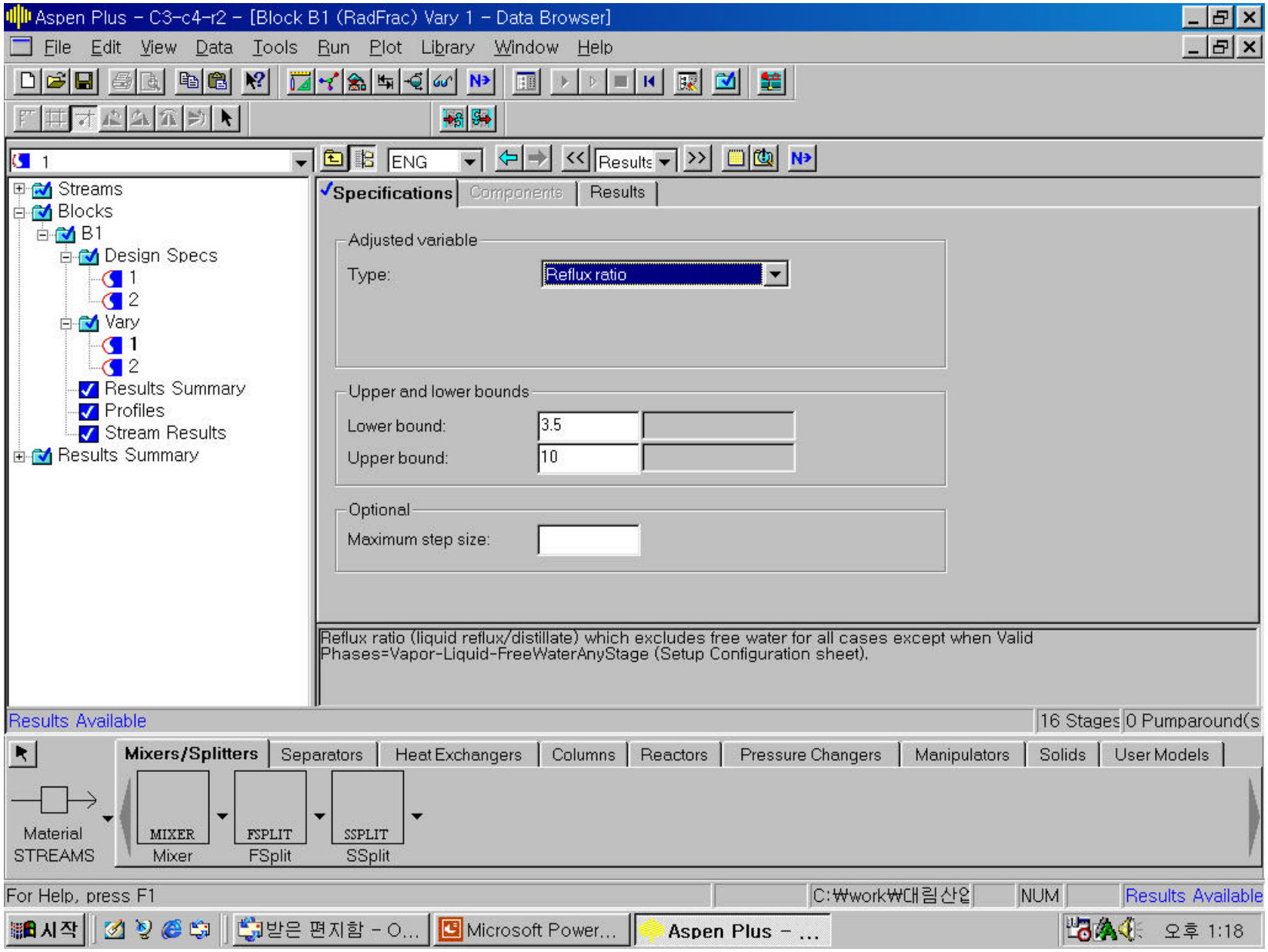
RadFrac (Design Spec 1)



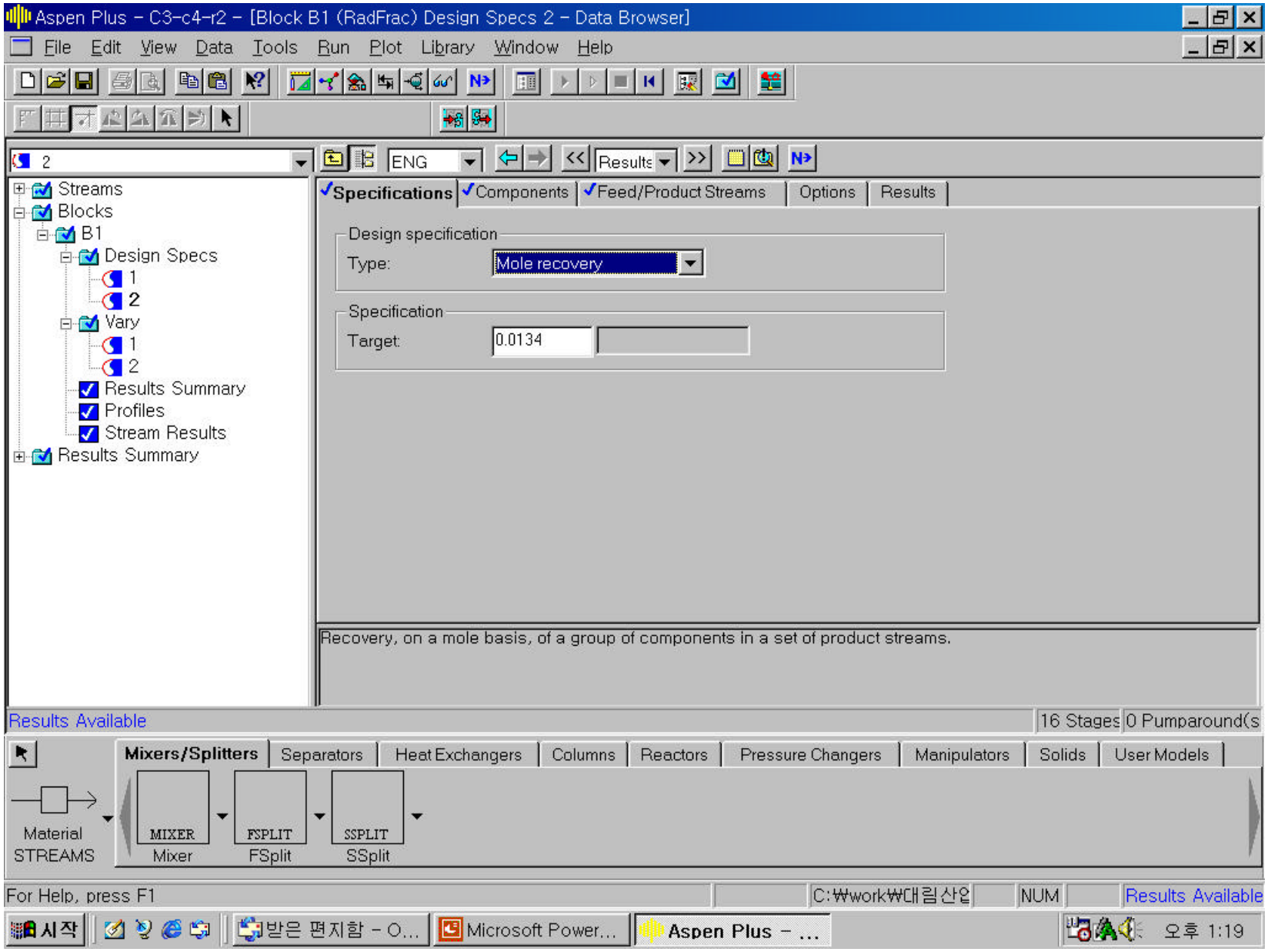
RadFrac (Design Spec 1)



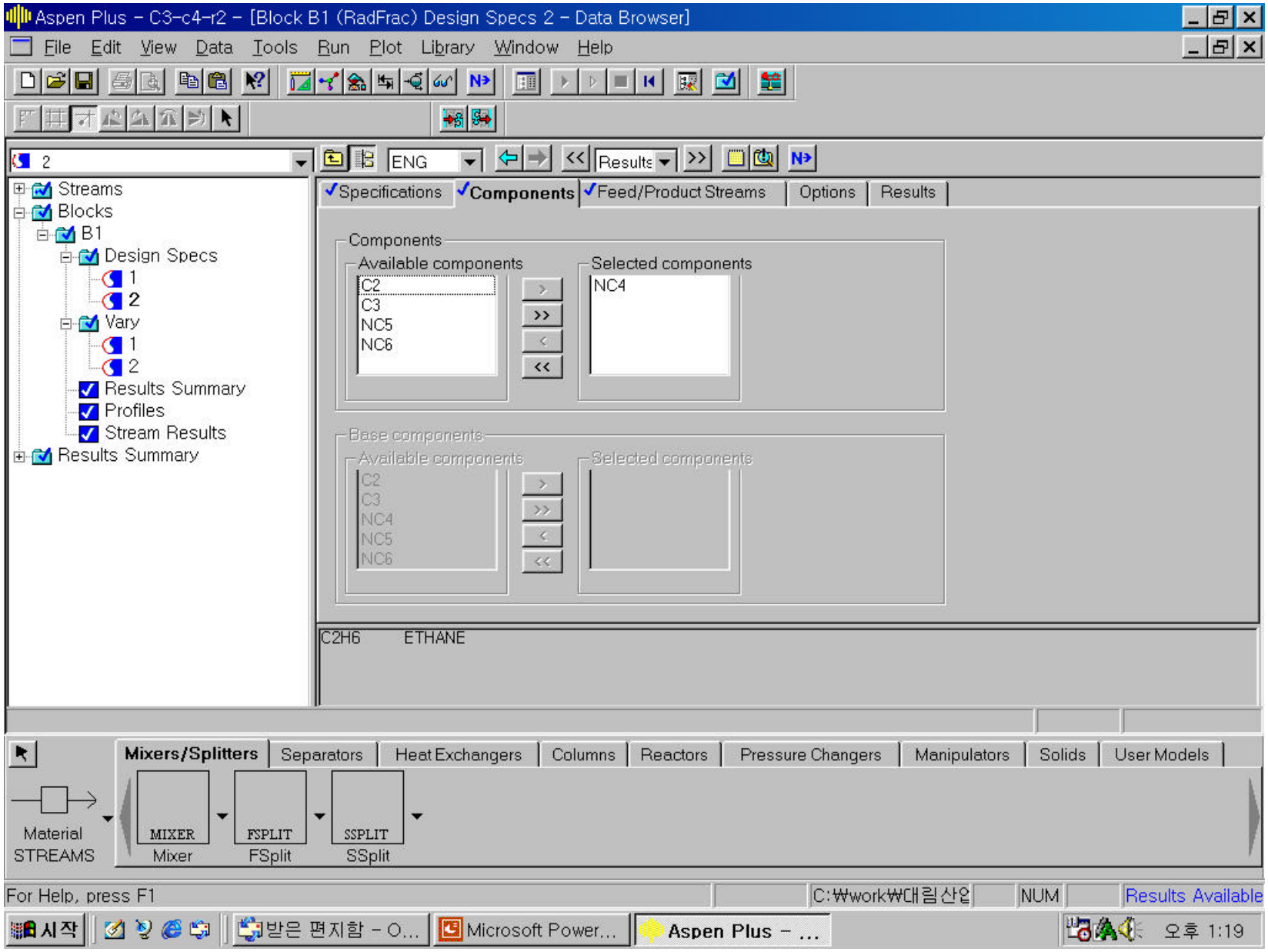
RadFrac (Variable 1)



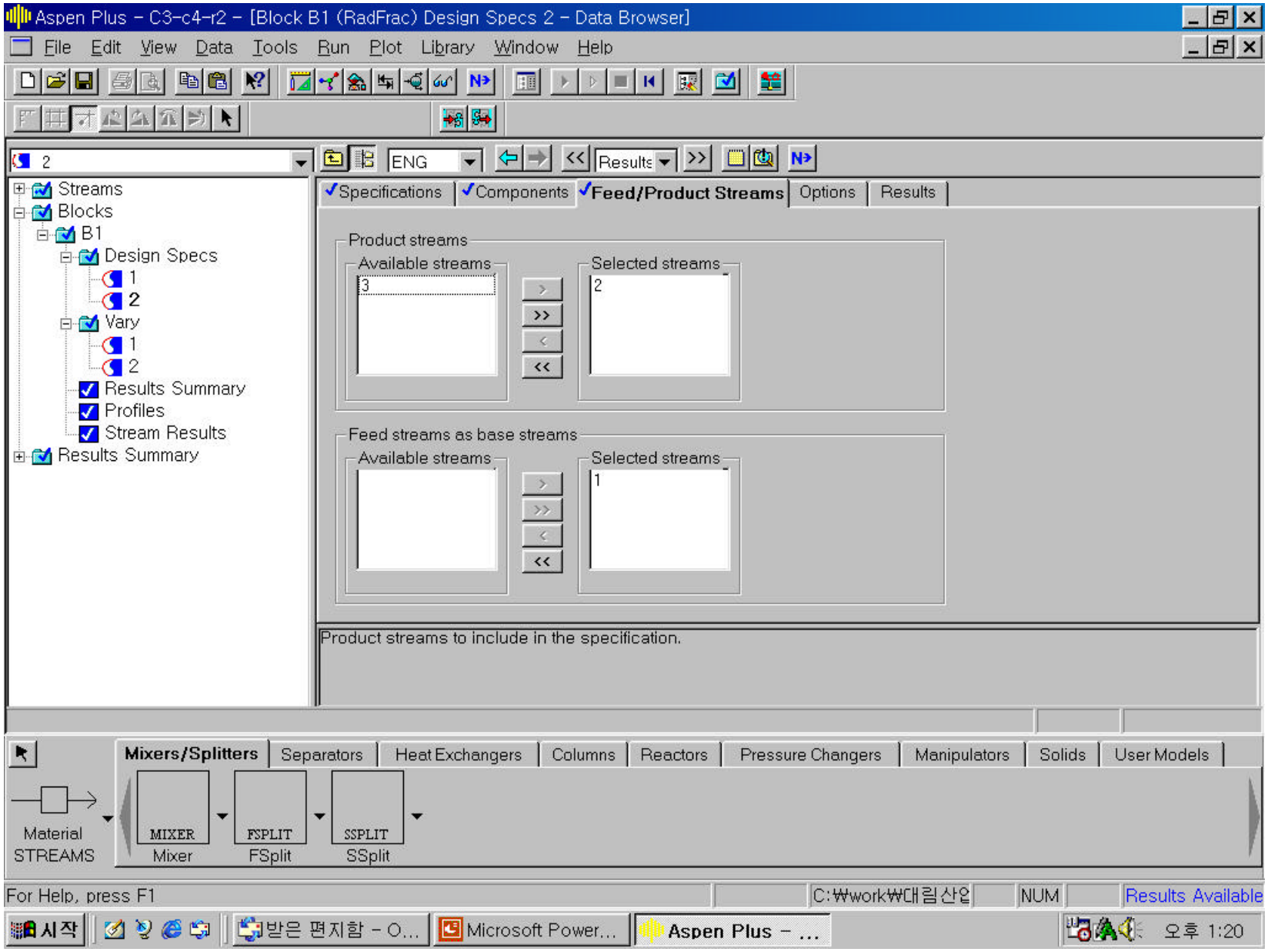
RadFrac (Design Spec 2)



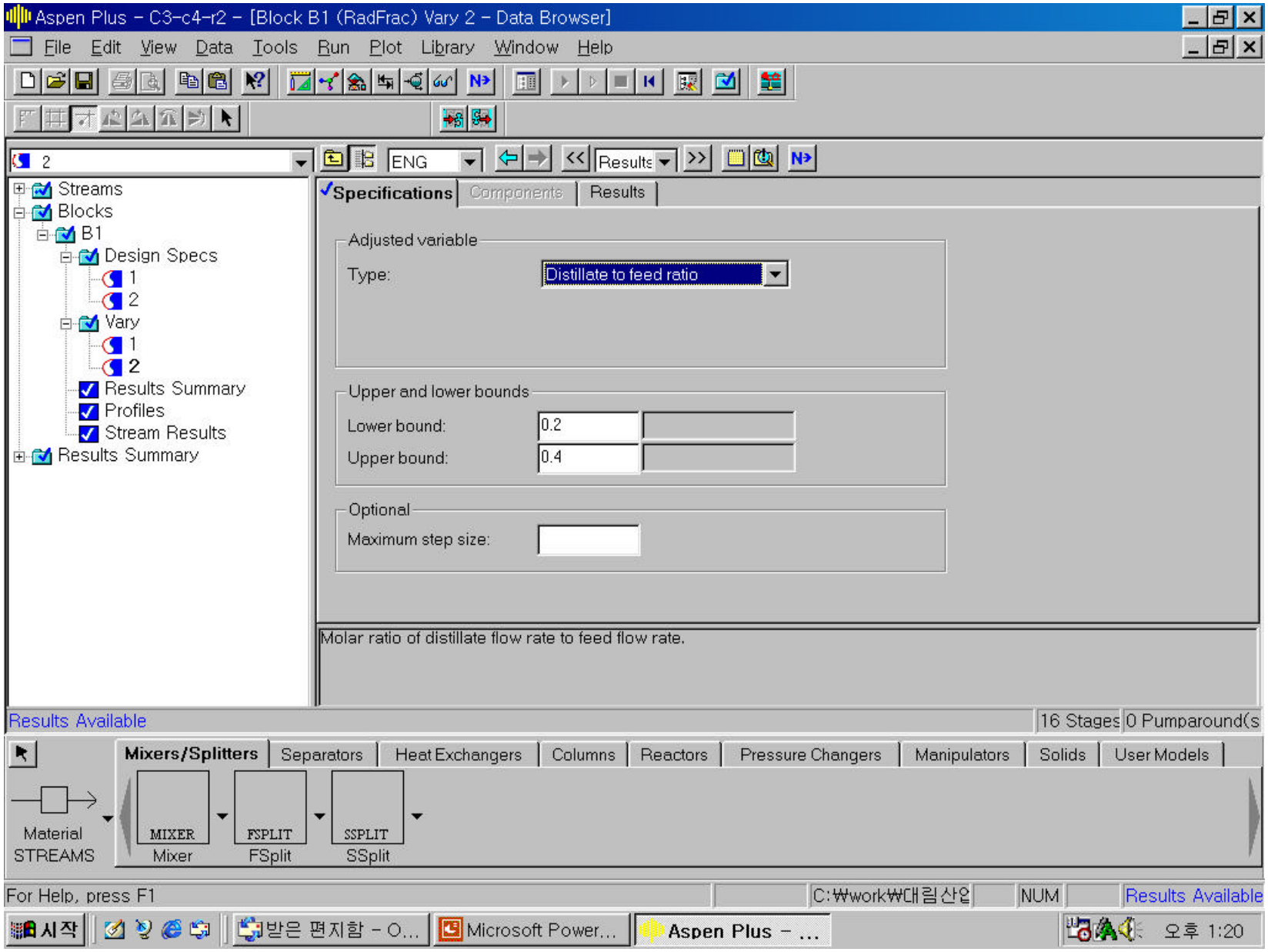
RadFrac (Design Spec 2)



RadFrac (Design Spec 2)



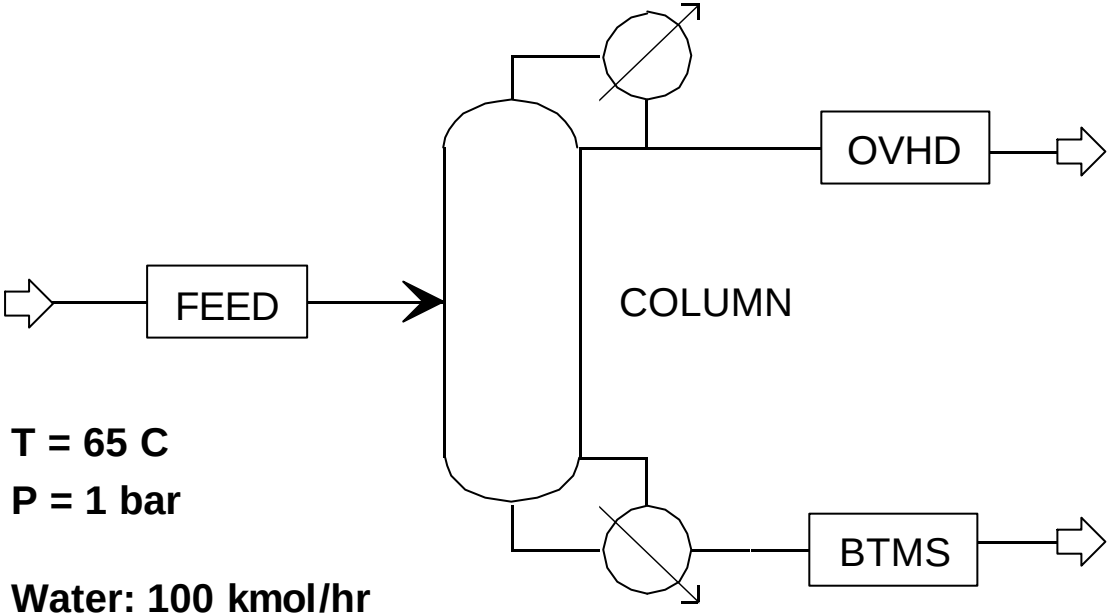
RadFrac (Variable 2)



Comparison between ‘ DSTWU’ , ‘ DISTIL’ , ‘ RadFrac1’ & ;RadFrac2’

	DSTWU	DISTIL	RadFrac1	RadFrac2
Reflux Ratio	5.7	5.7	5.7	9.14
Number of Tray	16	16	16	16
Feed Tray Location	9	9	9	9
Condenser Temperature	130 ºF	134 ºF	135.3 ºF	130 ºF
Condenser Heat Duty	-6.79	-6.94	-7.11	-10.95
Reboiler Heat Duty	9.06	9.63	9.79	13.67
C3 Recovery at Top	95.5 %	93.0 %	92.0 %	95.5 %
NC4 Recovery at Top	1.34 %	2.7 %	3.22 %	1.34 %

Methanol-Water RadFrac Column



T = 65 C
P = 1 bar

Water: 100 kmol/hr
Methanol: 100 kmol/hr

RadFrac specifications

- **Total Condenser**
- **Kettle Reboiler**
- **9 Stages**
- **Reflux Ratio = 1**
- **Distillate to feed ratio = 0.5**
- **Column pressure = 1 bar**
- **Feed stage = 6**

Use the NRTL-RK Property Method

Filename: RAD-EX.BKP

RadFrac Options

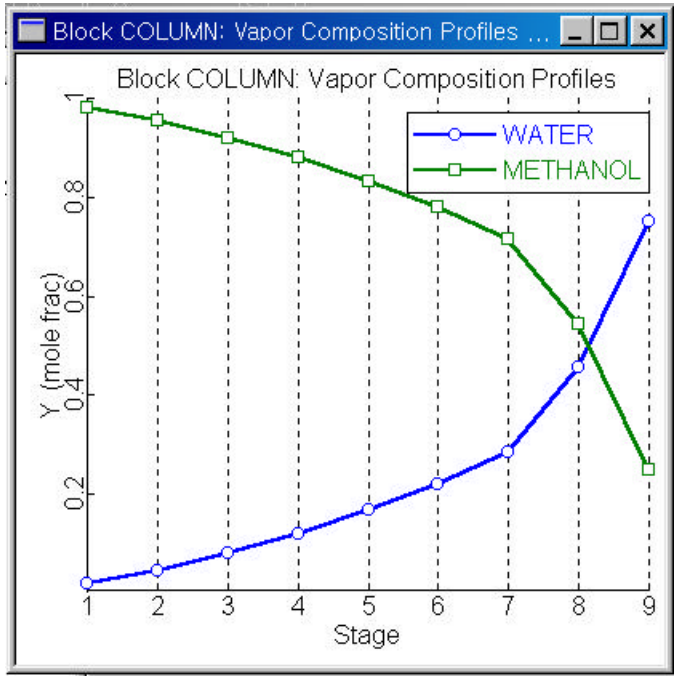
- To set up an absorber with no condenser or reboiler, set condenser and reboiler to none on the *RadFrac Setup Configuration* sheet.
- Either Vaporization or Murphree efficiencies on either a stage or component basis can be specified on the *RadFrac Efficiencies* form.
- Tray and packed column design and rating is possible.
- A Second liquid phase may be modeled if the user selects Vapor-liquid-liquid as Valid phases.
- Reboiler and condenser heat curves can be generated.

Plot Wizard

- Use Plot Wizard (on the Plot menu) to quickly generate plots of results of a simulation. You can use Plot Wizard for displaying results for the following operations:
  - Physical property analysis
  - Profiles for all separation models RadFrac, MultiFrac, PetroFrac and RateFrac
- Click the object of interest in the Data Browser to generate plots for that particular object.
- The wizard guides you in the basic operations for generating a plot.
- Click on the Next button to continue. Click on the Finish button to generate a plot with default settings.

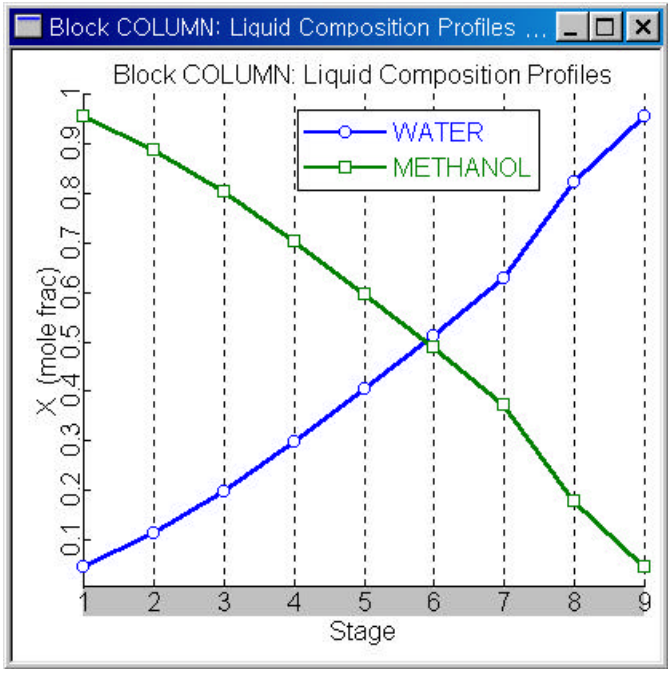
Plot Wizard Demonstration (1)

- Use the plot wizard on the column to create a plot of the *vapor phase compositions* throughout the column.



Plot Wizard Demonstration (2)

- Use the plot wizard on the column to create a plot of the *liquid phase compositions* throughout the column.



RadFrac DesignSpecs and Vary

- Design specifications can be specified and executed inside the RadFrac block using the *DesignSpecs* and *Vary* forms.
- One or more RadFrac inputs can be manipulated to achieve specifications on one or more RadFrac performance parameters.
- The number of specs should, in general, be equal to the number of varies.
- The DesignSpecs and Varys in a RadFrac are solved in a "Middle loop." If you get an error message saying that the middle loop was not converged, check the DesignSpecs and Varys you have entered.

RadFrac Convergence Problems

If a RadFrac column fails to converge, doing one or more of the following could help:

1. Check that physical property issues (choice of Property Method, parameter availability, etc.) are properly selected.

2. Ensure that column operating conditions are feasible.

3. If the column err/tol is decreasing fairly consistently, increase the maximum iterations on the *RadFrac Convergence Basic* sheet.

RadFrac Convergence Problems

(Continued)

4. Provide temperature estimates for some stages in the column using the *RadFrac Estimates Temperature* sheet (useful for absorbers).

5. Provide composition estimates for some stages in the column using the *RadFrac Estimates Liquid Composition* and *Vapor Composition* sheet (useful for highly non-ideal systems).

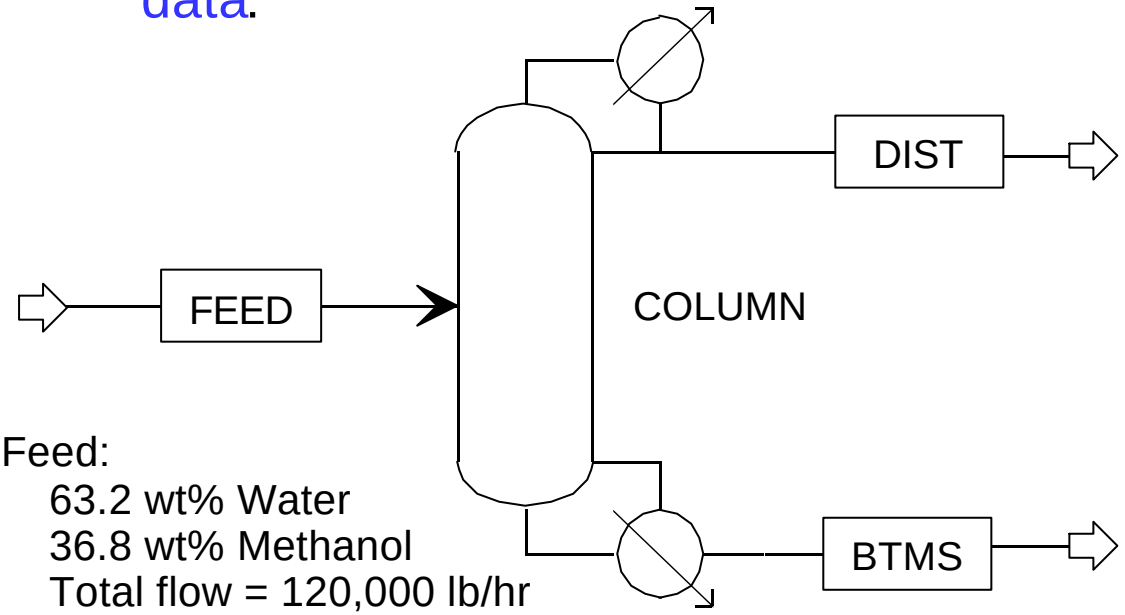
6. Experiment with different convergence methods on the *RadFrac Setup Configuration* sheet.

>> When a column does not converge, it is usually beneficial to Reinitialize after making changes.

RadFrac Workshop

Part A:

- Perform a rating calculation of a Methanol tower using the following data:



Column specification:
- 38 trays (40 stages)
- Feed tray = 23 (stage 24)
- Total condenser
- Top stage pressure = 16.1 psia
- Pressure drop per stage = 0.1 psi
- Distillate flowrate = 1245 lbmol/hr
- Molar reflux ratio = 1.3

Feed:
- 63.2 wt% Water
- 36.8 wt% Methanol
- Total flow = 120,000 lb/hr
- Pressure 18 psia
- Saturated liquid

Use

1) Ideal Raoult' s Law
2) NRTL Property Method
3) NRTL-RK Property Method
4) RK-Soave Property Method

Filename: RADFRAC.BKP

RadFrac Workshop

(Continued)

Part B:

- Set up design specifications within the column so the following two objectives are met:
  - 99.95 wt% methanol in the distillate
  - 99.90 wt% water in the bottoms

- To achieve these specifications, you can vary the distillate rate (800-1700 lbmol/hr) and the reflux ratio (0.8-2). Make sure stream compositions are reported as mass fractions before running the problem. Note the condenser and reboiler duties:

Condenser Duty :_____

Reboiler Duty :_____

Heat Exchangers

- ***Objective:***

Introduce the unit operation models used for heat exchangers and heaters.

- ***Aspen Plus References:***
- *Unit Operation Models Reference Manual,* Chapter 3, Heat Exchangers

Heat Exchanger Blocks

- Heater - Heater or cooler
- HeatX - Two stream heat exchanger
- MHeatX - Multi-stream heat exchanger
- Hetran - Interface to B-JAC Hetran block
- Aerotran - Interface to B-JAC Aerotran block

Working with the Heater Model

The Heater block mixes multiple inlet streams to produce a single outlet stream at a specified thermodynamic state.

Heater can be used to represent:

- Heaters
- Coolers
- Valves
- Pumps (when work-related results are not needed)
- Compressors (when work-related results are not needed)

Heater can also be used to set the thermodynamic conditions of an outlet stream.

Heater Input Specifications

Allowed combinations:

- Pressure (or Pressure drop) and one of:
  - Outlet temperature
  - Heat duty or inlet heat stream
  - Vapor fraction
  - Temperature change
  - Degrees of sub-cooling or superheating
- Outlet Temperature or Temperature change and one of:
  - Pressure
  - Heat Duty
  - Vapor fraction

Heater Input Specifications *(Continued)*

For single phase use Pressure (drop) and one of:

- Outlet temperature
- Heat duty or inlet heat stream
- Temperature change

Vapor fraction of 1 means dew point condition,
0 means bubble point

Working with the HeatX Model

- HeatX can perform simplified or rigorous rating calculations.
- Simplified rating calculations (heat and material balance calculations) can be performed if exchanger geometry is unknown or unimportant.
- For rigorous heat transfer and pressure drop calculations, the heat exchanger geometry must be specified.

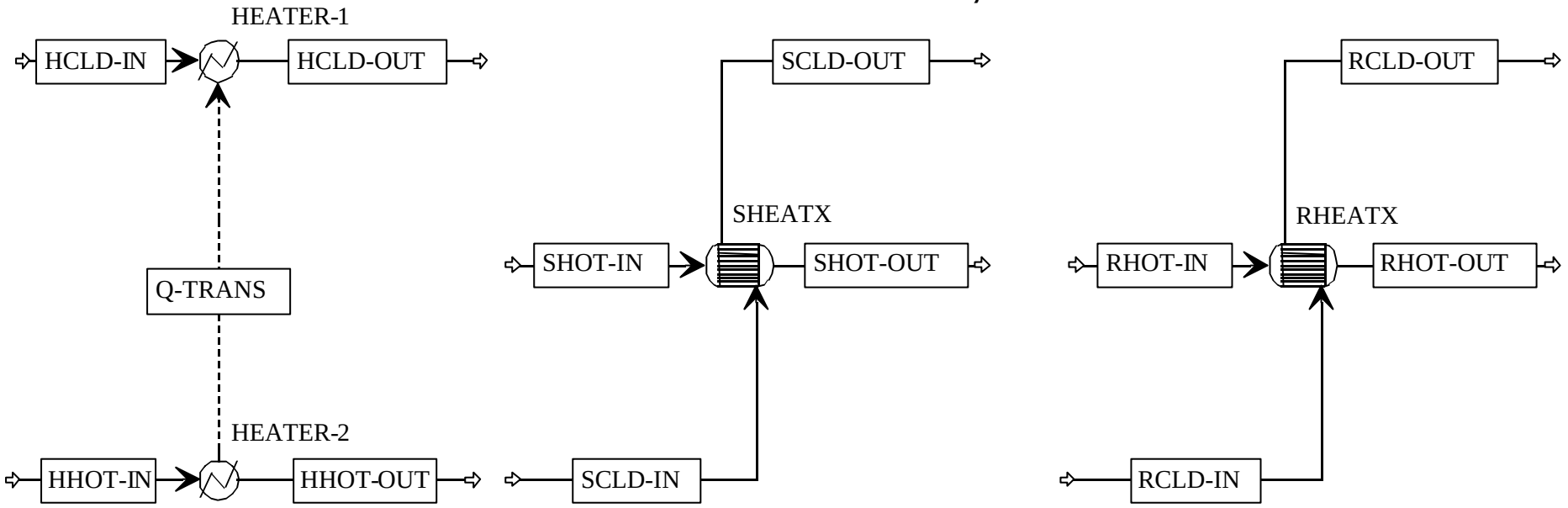
HeatX Workshop

Objective: Compare the simulation of a heat exchanger that uses water to cool a hydrocarbon mixture using three methods: a shortcut HeatX, a rigorous HeatX and two Heaters connected with a Heat stream.

- Hydrocarbon stream
  - Temperature: 200 C
  - Pressure: 4 bar
  - Flowrate: 10000 kg/hr
  - Composition: 50 wt% benzene, 20% styrene, 20% ethylbenzene and 10% water
- Cooling water
  - Temperature: 20 C
  - Pressure: 10 bar
  - Flow rate: 60000 kg/hr
  - Composition: 100% water

HeatX Workshop *(Continued)*

When finished, save as filename: HEATX.BKP



Use the NRTL-RK Property Method for the hydrocarbon streams.

Specify that the valid phases for the hydrocarbon stream is Vapor-Liquid-Liquid.

Specify that the Steam Tables are used to calculate the properties for the cooling water streams on the Block BlockOptions Properties sheet.

Start with the General with Metric Units Template.

HeatX Workshop *(Continued)*

- Shortcut HeatX simulation:
  - Hydrocarbon stream exit has a vapor fraction of 0
  - No pressure drop in either stream
- Two Heaters simulation:
  - Use the same specifications as the shortcut HeatX simulation
- Rigorous HeatX simulation:
  - Hydrocarbons in shell leave with a vapor fraction of 0
  - Shell diameter 1 m, 1 tube pass
  - 300 bare tubes, 3 m length, pitch 31 mm, 21 mm ID, 25 mm OD
  - All nozzles 100 mm
  - 5 baffles, 15% cut
  - Create heat curves containing all info required for thermal design.
  - Change the heat exchanger specification to Geometry and re-run.

Pressure Changers

Objective:

Introduce the unit operation models used to change pressure: pumps, compressors, and models for calculating pressure change through pipes and valves.

Aspen Plus References:

Unit Operation Models Reference Manual, Chapter 6, Pressure Changers

Pressure Changer Blocks

- Pump - Pump
- Compr - Compressor or turbine
- MCompr - Multi-stage compressor or turbine
- Valve - Control valve or Pressure Let-down Valve
- Pipe - Single-segment pipe
- Pipeline - Multi-segment pipe

Reactor Models

Objective:

Introduce the various classes of reactor models available, and examine in some detail at least one reactor from each class

Aspen Plus References:

Unit Operation Models Reference Manual, Chapter 5, Reactors

Reactor Overview