

# CHE 654 Course Notes

(7<sup>th</sup> Edition: May 2014)

---

## Computer Applications for Chemical Engineering Practice



Dr. Hong-ming Ku

Chemical Engineering Practice School

King Mongkut's University of Technology Thonburi

1

---

## Process Simulation with ASPEN PLUS

---

CHE654 Course Notes

### Section 1: Introduction and ASPEN PLUS User Interface

These course materials are applicable to Version 8.4 of ASPEN PLUS

ASPEN PLUS™ is a trademark of Aspen Technology, Inc., Burlington, MA, U.S.A.

2

## What Are Process Simulation and Flowsheeting?

---

- ❑ The use of computer programs to help solve the characteristic equations and perform sizing and costing calculations of a chemical process
  - ❑ Process simulation uses underlying physical relationships such as
    - mass and energy balances
    - equilibrium relationships
    - reaction kinetics
    - conditions of unit operation models
- to predict plant operating conditions, product stream compositions, flows, and properties.

3

## Why Use Process Simulation?

---

- ❑ Huge savings in manpower and design cost
- ❑ Allows prediction of process behavior using mass and energy balances, and phase and chemical equilibrium
- ❑ Allows case studies and sensitivity studies (“what-if” analyses)
- ❑ Can perform optimization runs
- ❑ Consistent results in very presentable forms and formats
- ❑ Can perform economic evaluation and profitability of a design process

4

## History of ASPEN PLUS and Aspen Technology Inc.

---

- ❑ ASPEN = Advanced System for Process Engineering  
→ Steady-State Simulator
- ❑ Initially funded by the US Department of Energy (DOE) in 1975 to develop a process simulation program to handle solids
- ❑ ASPEN project was contracted to MIT and completed in 1980  
End Product = ASPEN (Public Version)
- ❑ Aspen Technology Inc. (AspenTech) was founded in 1981 to enhance and debug ASPEN  
End Product = ASPEN PLUS

5

## Key Features of ASPEN PLUS

---

- ❑ Easy to use Graphical User Interface (GUI)
- ❑ Comprehensive and robust set of unit operation models
- ❑ Complete set of physical property models and equations
- ❑ Property analysis, e.g. property curves such as vapor pressure vs. **T**, phase envelopes, **T-xy**, and **P-xy** plots
- ❑ Databanks for pure components, aqueous systems, solids, and binary pairs

6

## Key Features of ASPEN PLUS (Cont'd)

---

- Data regression system, property estimation system, and databank management system
- Characterization and simulation of petroleum including a dedicated unit operation model
- Unique and rigorous simulation of electrolytes
- Solids handling capabilities including unit operations
- Feedback and feed-forward control capabilities

7

## Key Features of ASPEN PLUS (Cont'd)

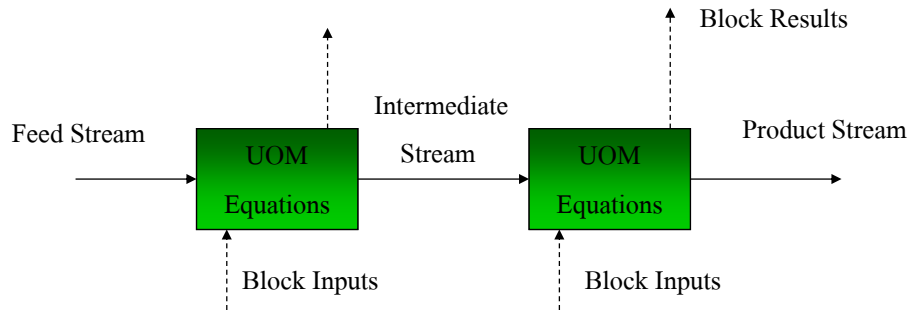
---

- Automatic flowsheet sequencing and convergence
- Sensitivity and case-study analysis
- State-of-the-art optimization capabilities
- Add-on modules such as bioprocessing unit operations and polymer processing
- Useful interfacing features

8

## Sequential Modular Approach (SMA)

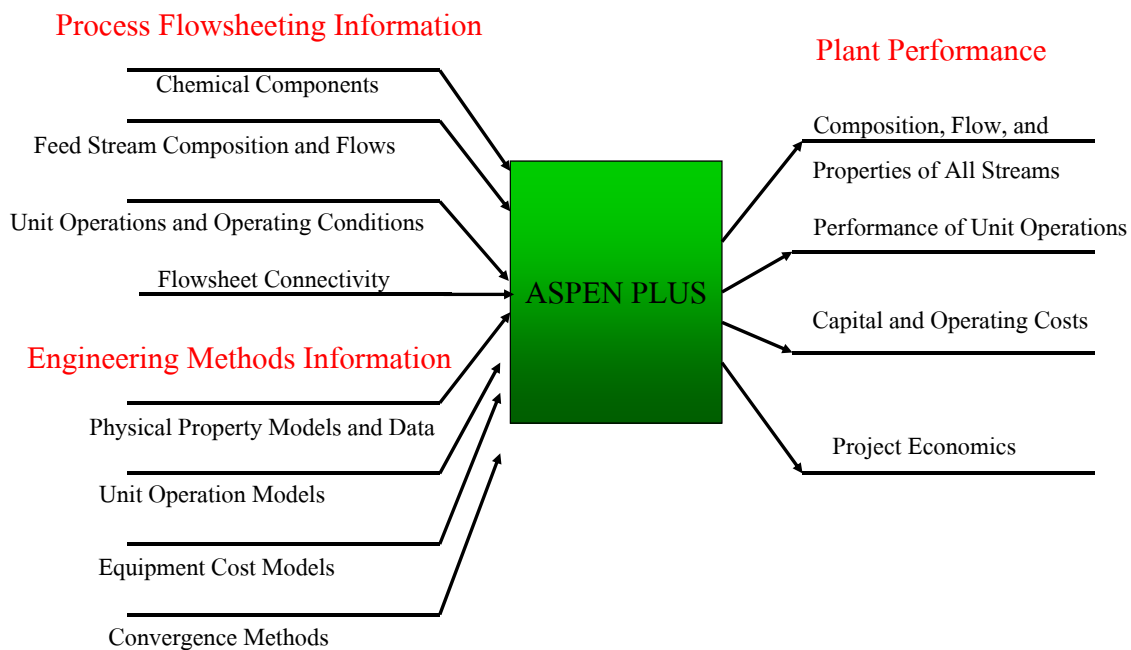
- ❑ ASPEN PLUS is primarily a sequential modular simulator.
- ❑ Flow of Information



- ❑ **One-block-at-a-time sequential execution:** outlet stream result are used as input to the next block in the sequence

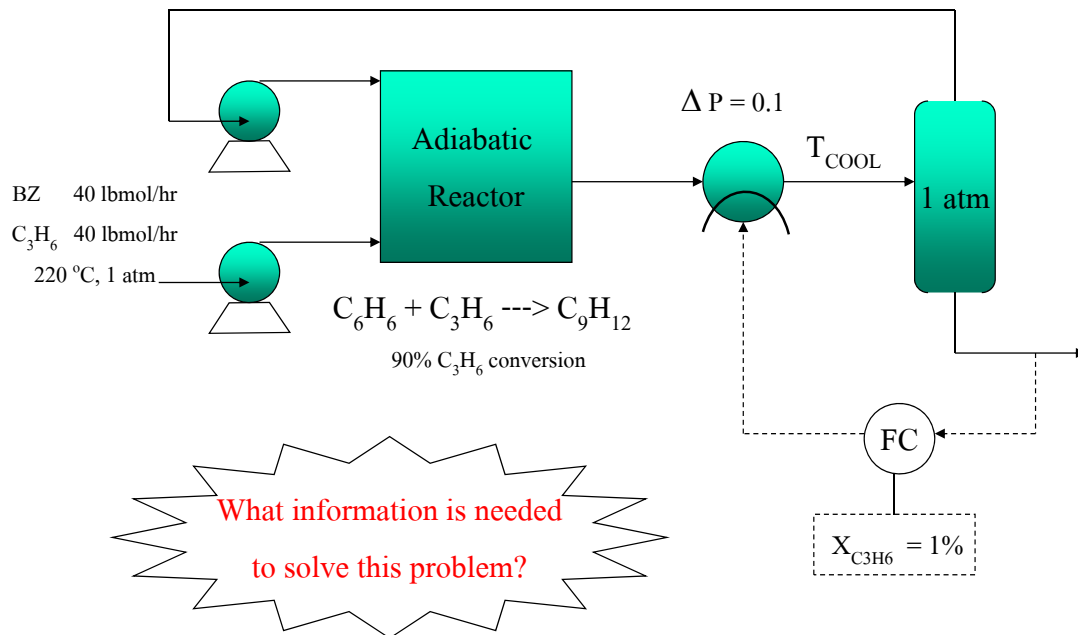
9

## Flow of Information in a SMA Simulator



10

# A Simulation Example Problem



11

## Introduction to ASPEN PLUS User Interface

□ GUI consists of 2 main components

### 1. Graphics

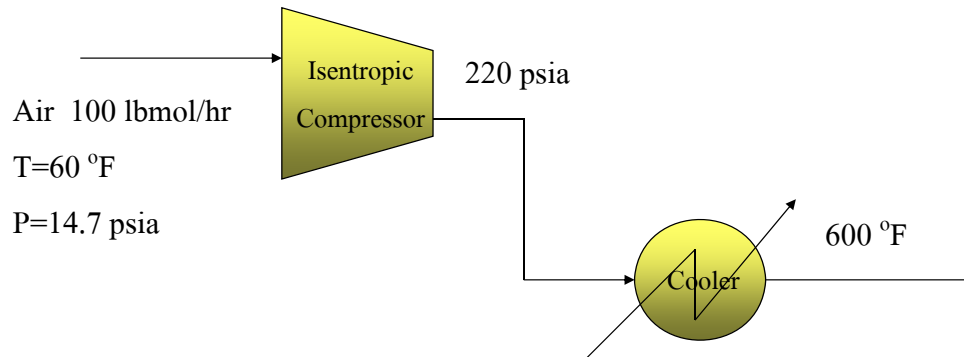
- Flowsheet graphics
- Results plots
- Process flow diagrams (PFD) generation

### 2. Forms and Menus

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

12

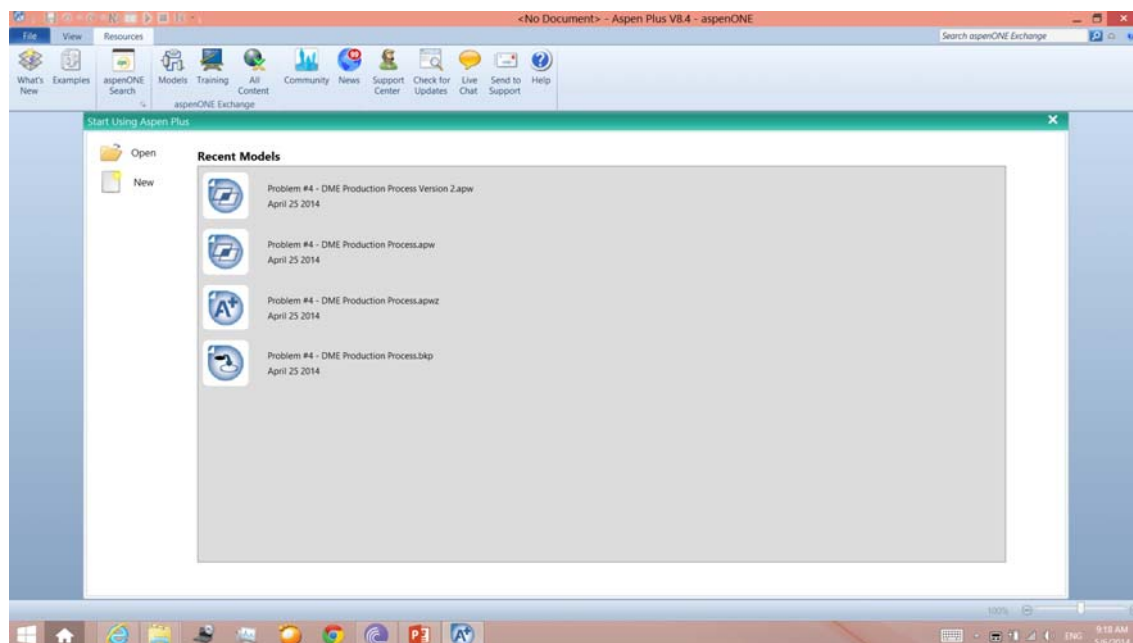
## Example Problem: Compression and Cooling of Air



Physical property calculations: Ideal Gas vs. Redlich-Kwong-Soave

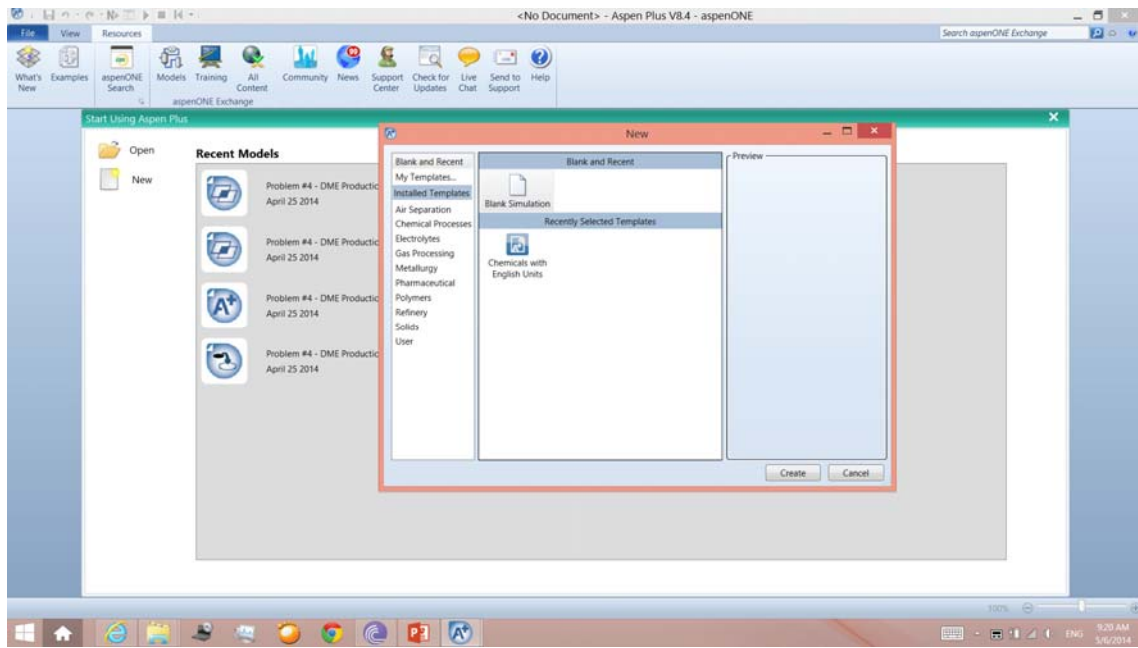
13

## ASPEN PLUS User Interface Startup



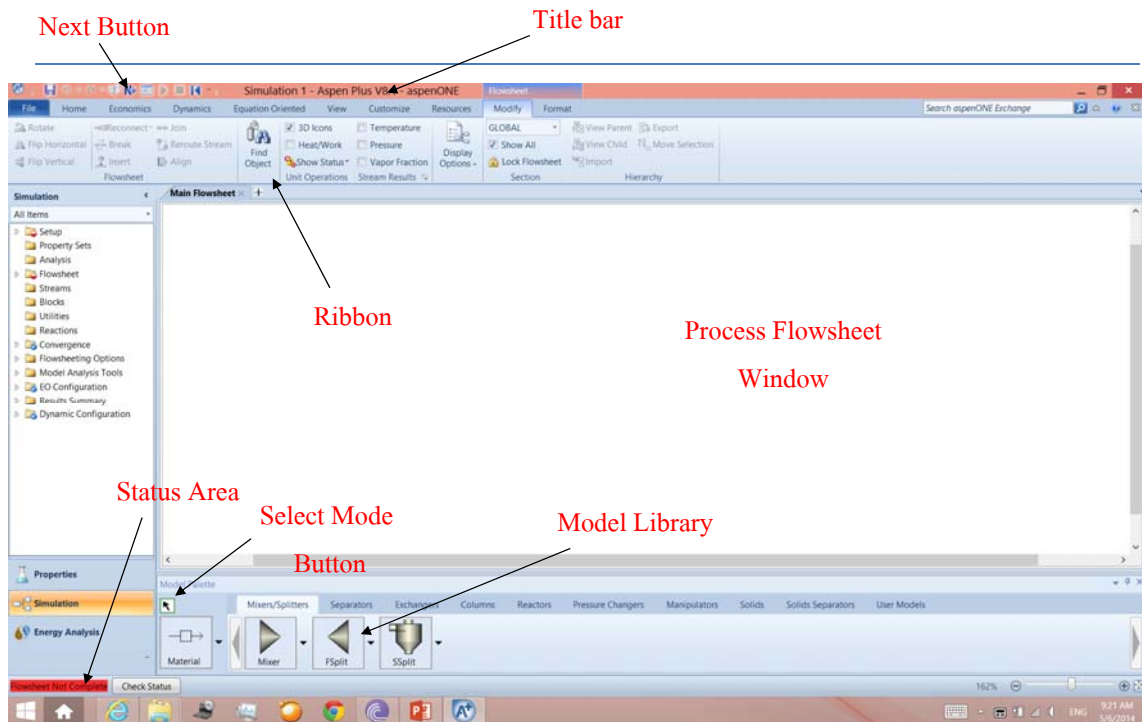
14

# ASPEN PLUS User Interface Startup Template



15

# ASPEN PLUS Main Window



16



## ASPEN PLUS Main Window (Cont'd)

Window Part	Description
Title bar	Horizontal bar at top of window that displays the Run ID. Simulation 1 is the default ID until you give the run a new name.
Ribbon	A new user interface command paradigm that contains major features of an application.
Next Button	Invokes the Aspen Plus expert system. Guides you through the steps required to complete your simulation.
Status Area	Displays status information about the current run.
Scroll bars	The vertical and horizontal bars, located on the right and bottom of the Process Flowsheet Window. They are used to scroll through a flowsheet or a list that is too large to be viewed on the screen all at once.

## How to Use the Mouse Buttons in GUI

---

### ☐ Left Button:

1. Select menu, command, option, or object
2. Place a block
3. Confirm an action
4. Unselect an object by clicking away from that object
5. Define area for zooming or resizing by click, drag, and release of left button

### ☐ Right Button:

1. Display popup menu
2. Cancel an action

## How to Open, Save, and Exit a Run

---

- ❑ Click on the File Pulldown menu

Some Important Options:

- New** => Clears workspace and starts a new run
- Open** => Opens an existing run
- Save / Save As** => Saves this run without exiting
- Print** => Prints the active window
- Exit** => Leaves ASPEN PLUS

19

## Five Essential Elements in a Simulation Run

---

- ❑ The following 5 elements must always be specified in a simulation:
  1. **Setup** - specifies basic information for a run, such as unit of measurements, run type, report options, etc.
  2. **Components** - identifies all chemical species in the simulation
  3. **Physical Properties** - specifies physical property methods and models to compute stream properties such as enthalpy, entropy, molar volume, temperature, etc.
  4. **Streams** - specifies input for feed streams, such as temperature, pressure, composition, etc.
  5. **Blocks** - specifies conditions or input for unit operation blocks

20

## Five Essential Elements (Cont'd)

Setup

Identify Components

Specify Property Methods

GUI is divided into Properties and Simulation

Component ID	Type	Component name	Alias
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2

21

## Five Essential Elements (Cont'd)

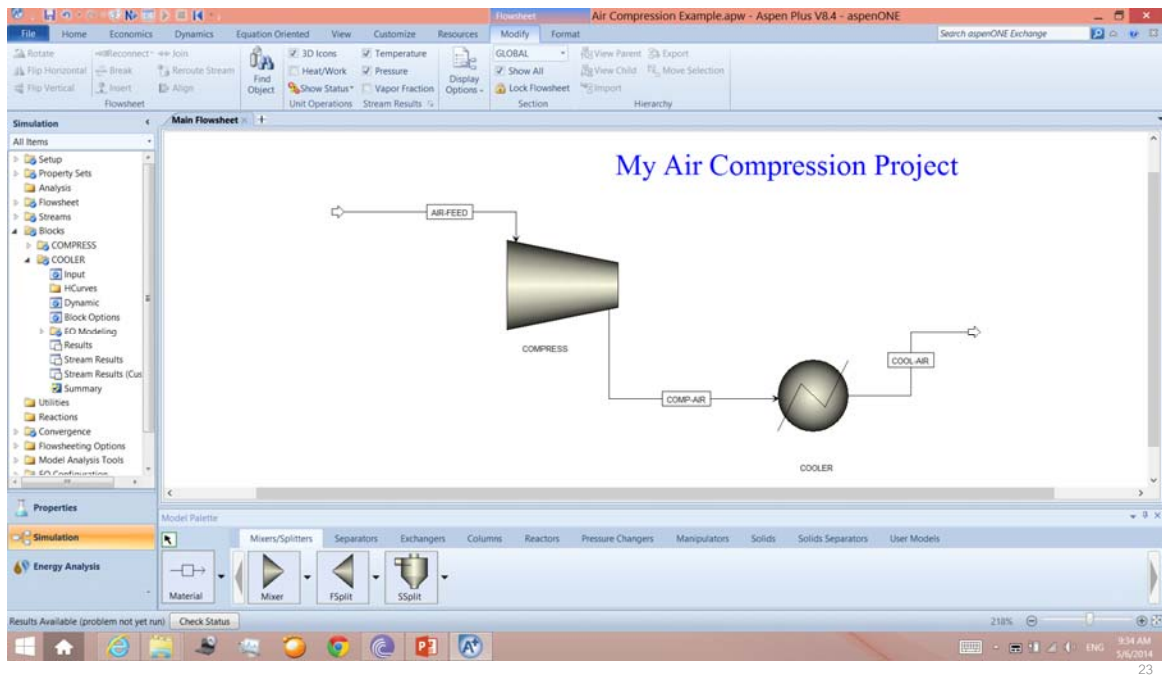
Specify Streams

Specify Blocks

Air Compression Example				
Stream ID	AIR-FEED	COMP-AIR	COOL-AIR	
Temperature	F	60.0	670.4	600.0
Pressure	psia	14.70	220.00	220.00
Vapor Frac		1.000	1.000	1.000
Mole Flow	Bmol/hr	100.000	100.000	100.000
Mass Flow	lb/hr	2885.040	2885.040	2885.040
Volume Flow	cuft/hr	37928.442	6527.137	5203.502
Enthalpy	MMBtu/hr	-0.012	0.572	0.371
Mole Flow	Bmol/hr			
N2		79.000	79.000	79.000
O2		21.000	21.000	21.000

22

## Example Problem: Compression and Cooling of Air



## Air Compression Problem: Setup Sheet

The screenshot shows the "Setup" sheet in Aspen Plus V8.4 - aspenONE. The "Global" tab is active, displaying simulation parameters for the "Air Compression Example". The parameters are as follows:

- Title: Air Compression Example
- Global unit set: ENG
- Input mode: Steady-State
- Stream class: **CONVEN** (Annotated: "Always CONVEN for V-L systems")
- Flow basis: Mole
- Ambient pressure: 14.6959 psi
- Ambient temp: 50 F
- Valid phases: **Vapor-Liquid** (Annotated: "Phases expected in the simulation")
- Free water: No
- Operational year: 8766 hr

Annotations include:

- "Always CONVEN for V-L systems" pointing to the Stream class dropdown.
- "Phases expected in the simulation" pointing to the Valid phases dropdown.
- "Data Browser Menu Tree" pointing to the left-hand navigation pane.

Text on the right side of the sheet reads: "To establish defaults that apply to the entire simulation".

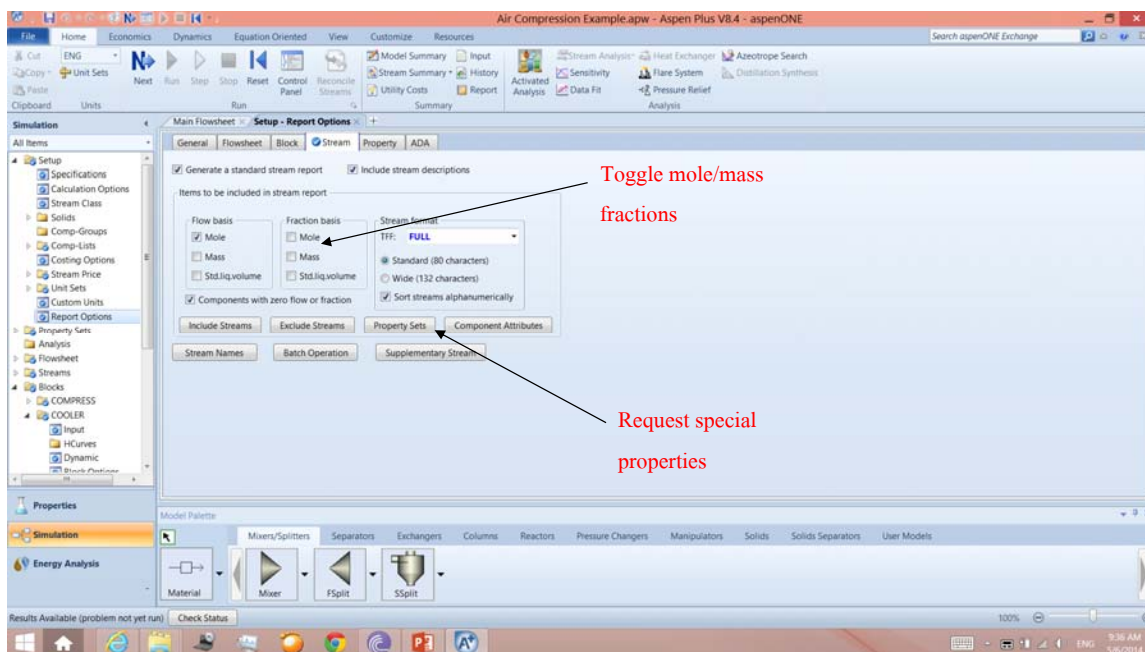
## Setup Sheet (Cont'd)

### □ Report Options

- Used to customize how simulation results and reports should look
- For example, stream results can be customized to show mole fractions and mass fractions.
- Streams can also be customized to include special properties, such as viscosity, thermal conductivity, Reynolds numbers, etc.

25

## Setup Report Options Sheet for Streams



26

# Status Indicators for Forms and Sheets

**Status Indicators**

Status indicators display the completion status for the entire simulation as well as for individual forms and sheets. The status indicators appear:

- Next to sheet names on the tabs of a form
- As symbols representing forms in the navigation pane
- On the flowsheet (warning and error icons)
- In the context menu when right-clicking a stream or block, next to the **Input** and **Results** commands

This table shows the meaning of the symbols that appear:

Icon Symbol	On a(n)	Means
[Green Checkmark]	Input form or sheet	Required input complete, or visited and no data required **
[Red X]	Input form or sheet	Required input incomplete
[White]	Input form	No data entered
[Blue]	Mixed form	Input and results
[Blue]	Results form	No results present (calculations have not been run)
[Green]	Results form	Results available without Errors or Warnings (OK) **
[Yellow]	Results form or flowsheet	Results available with Warnings **
[Red]	Results form or flowsheet	Results available with Errors **
[Red]	Results form	Results inconsistent with current input (input changed)
[White]	Input folder	No data entered
[Red X]	Input folder	Required input incomplete
[Green Checkmark]	Input folder	Required input complete, or visited and no data required **
[White]	Results folder	No results present
[Green]	Results folder	Results available - OK **
[Yellow]	Results folder	Results available with Warnings **
[Red]	Results folder	Results available with Errors **
[Red]	Results folder	Results inconsistent with current input (input changed)
[Grey]	Folder or form	Object deactivated

\* The required input complete icons [Green Checkmark], [Blue], and [Green] appear on some forms and folders in the navigation pane where no input is required as soon as you enter the form. You can restore these to the no data entered icon by right-clicking the icon and selecting **Delete**. In this case, the form or folder will not be deleted, but it will be restored to its original status in a blank simulation.

\*\* The OK, Warning, or Error status indicator ignores EO synchronization status when the **Method** is **Sequential Modular**. When it is **Equation Oriented**, an EO synchronization failure is treated as an Error.

In addition to these symbols, if you place the mouse pointer over one of the forms or folders in the navigation pane, a tooltip will appear showing the status in text. This status includes additional information which may

# Components Specifications Sheet

**Components - Specifications**

Component ID	Type	Component name	Alias
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2

Annotations:

- Arrows point to the **N2** and **O2** Component IDs with the text: **User-defined unique names**
- Arrows point to the **Conventional** Type with the text: **Always, for V-L components**
- Arrows point to the **NITROGEN** and **OXYGEN** Component names with the text: **Names and formulae as appeared in the databanks**

To identify chemical components in the simulation so A+ can pick up their properties from databanks

# Properties Specifications Sheet

Default to base method

Identify Henry's components

Based method for simulation

Used only for electrolytes

Contain defaults

To specify global property methods and models for your simulation

## Properties Specifications Sheet (Cont'd)

❑ An ASPEN PLUS property method contains equations and correlations

to calculate the following:

- Enthalpy, entropy, fugacities, molar volume, transport properties (e.g. surface tension, viscosity), etc.
- Used for mass and energy calculations

❑ For each simulation run, you must:

- Select a primary property method (e.g. IDEAL)
- Identify any components to be treated as Henry's components for certain class of property methods (Henry's components are light gases which are dissolved in the liquid phase.)

## Feed Stream Specifications

---

❑ Used to specify the thermodynamic and flow conditions of a feed stream

❑ For conventional components (i.e. vapor-liquid):

The Substream name is always MIXED.

❑ Specifying the state variables (stream condition):

- Temperature, Pressure, and Vapor Fraction
- Pick a combination of 2 state variables out of 3
- Vapor Fraction = 1 ---> saturated vapor (vapor at its dew point)
- Vapor Fraction = 0 ---> saturated liquid (liquid at its bubble point)
- $0 < \text{Vapor Fraction} < 1$  ---> mixed phase or two-phase stream

31

## Feed Stream Specifications (Cont'd)

---

❑ Two options to enter feed flow rates

1. Specify the total flow and the composition (e.g. mole fractions, mass fractions)
2. Specify individual component flow rates.

❑ Several basis for Total Flow:

- Mass, Mole, Volume, and Standard Liquid Volume (STDVOL)
- Standard liquid volume is defined at 60 °F and 1 atmosphere

32

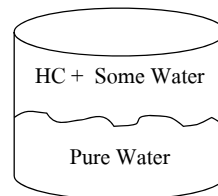
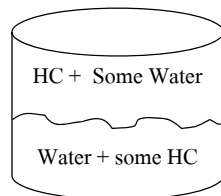


# Feed Stream Specifications (Cont'd)

## Flash Options Sheet (Optional)

- Specify the maximum number of iterations for flash calculations (default = 30)
- Specify error tolerance => relative error: how tightly the flash calculations should be converged (default = 0.0001)
- Specify valid phases => expected phases in the feed

## Liquid-Liquid vs. Liquid-Freewater



33

## Feed Stream Specifications - Total Flow Option

Flash Type: Temperature Pressure

State variables  
Temperature: 60 F  
Pressure: 14.7 psia

Vapor fractions:

Total flow basis: Mole  
Total flow rate: 100 lbmol/hr

Solvent:

Composition  
Mole-Flow lbmol/hr

Component	Value
N2	0.79
O2	0.21

Total: 1

Specify total flow

Specify composition in mole fractions

34

## Feed Stream Specifications - Component Flow Option

The screenshot shows the 'AIR-FEED (MATERIAL)' specifications window. The 'Composition' table is as follows:

Component	Value
N2	79
O2	21
Total	100

An arrow points to the table with the text: **Specify individual component flows**

35

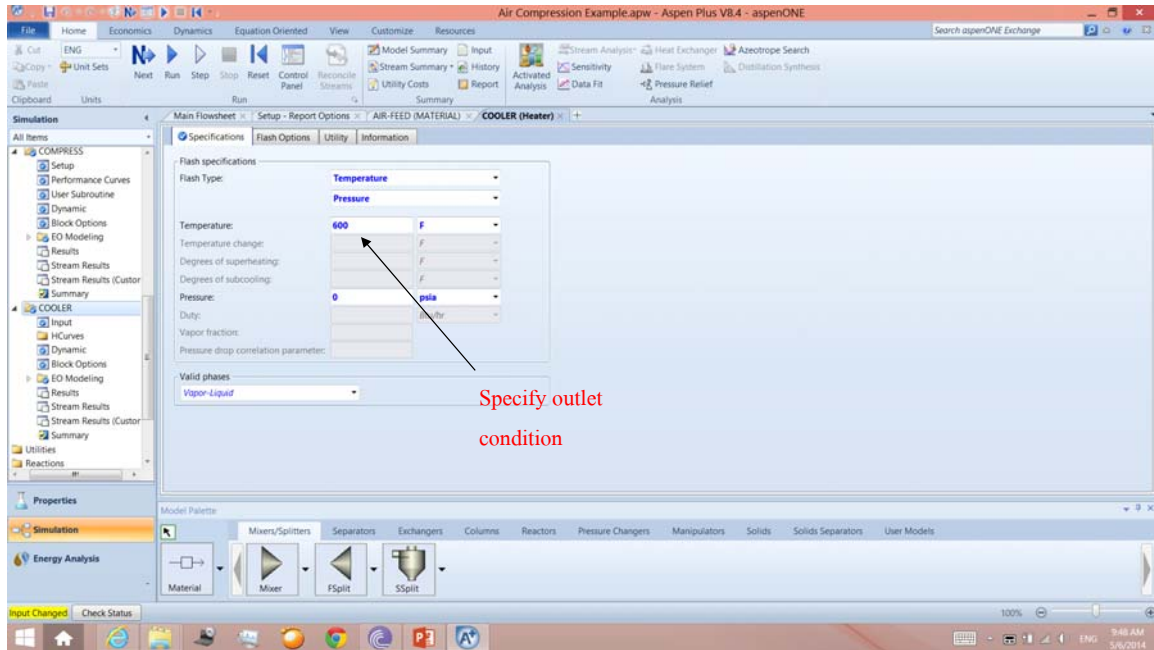
## Unit Operation Block Specifications (COMPR)

The screenshot shows the 'COMPRESS (Compr)' specifications window. The 'Model and type' section shows 'Compressor' selected and 'Isentropic' type. The 'Outlet specification' section shows 'Discharge pressure' set to 220 psia. Arrows point to these fields with labels: **Specify compressor type**, **Specify outlet condition**, and **Optional**.

To specify the operating conditions of each unit operation block in the flowsheet

36

## Unit Operation Block Specifications (HEATER)



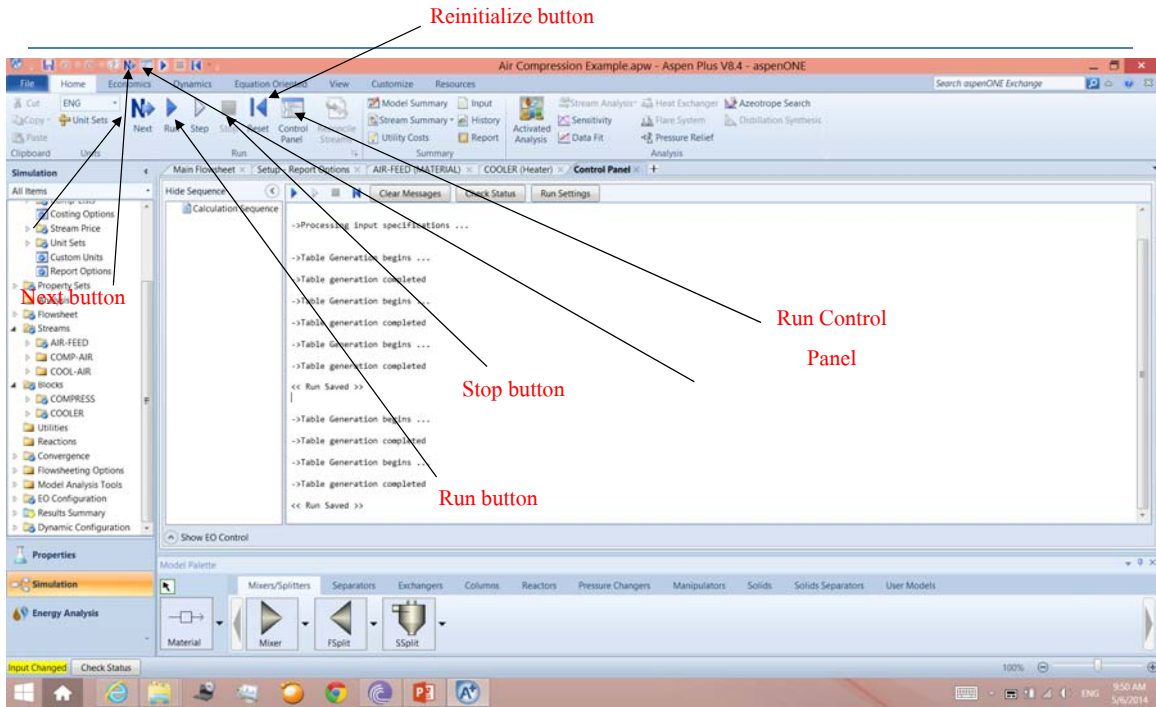
37

## Making an ASPEN PLUS Run

- ❑ ASPEN PLUS is ready to run when the Status Area says “Required Input Complete”.
- ❑ Click the Next Button to run.
- ❑ Other ways to run ASPEN PLUS
  1. Press the Run Button.
  2. Press F5.
- ❑ The Reinitialize Button will purge all simulation results and reinitialize calculations.

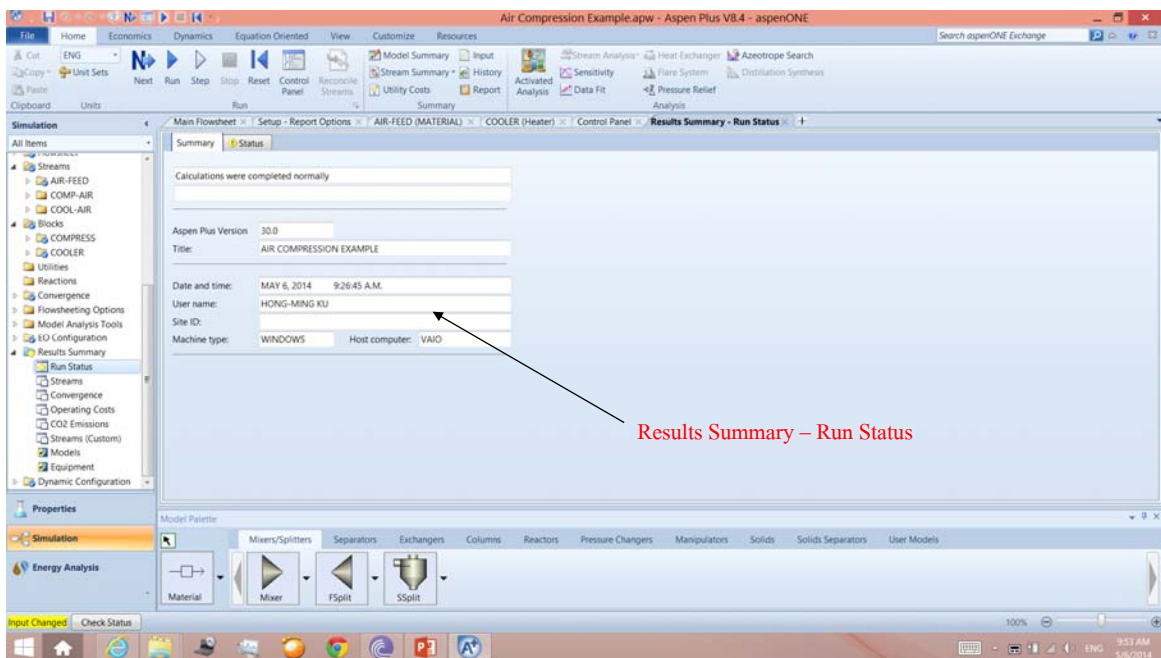
38

# ASPEN PLUS Control Panel



39

# Checking Simulation Results



40

## Comparing Results: IDEAL vs. RK-SOAVE

---

	<u>IDEAL Method</u>	<u>RK-SOAVE Method</u>
Compressed Air Temp	870.08 ° F	870.43 ° F
Compressor HP	228.85 HP	229.48 HP
Cooler Duty	-0.19976E+6	-0.20074E+6

- ☐ IDEAL and RK-SOAVE gave very similar results. So IDEAL is an acceptable property method for this simulation.

41

## Workshop 1: Flashing of Light Hydrocarbons

---

- ☐ Recap everything we've learned so far with our first workshop
- ☐ Go to Course Notes Section 9 and work on Workshop 1



42