CHE 654 Course Notes

(7th Edition: May 2014)

Computer Applications

for

Chemical Engineering Practice

Dr. Hong-ming Ku

Chemical Engineering Practice School

King Mongkut's University of Technology Thonburi

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

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.

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

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

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

Key Features of ASPEN PLUS (Cont'd)

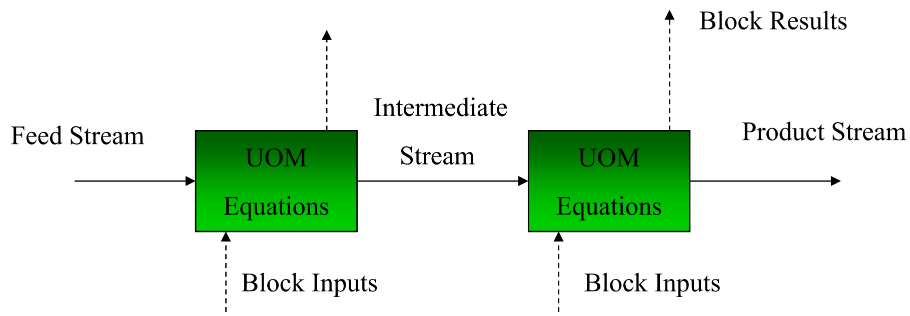
- Data regression system, property estimation system, and databank management system
- Characterization and simulation of petroleum including a dedicated unit operation model
- Unique and rigorous simulation of electrolytes
- Solids handling capabilities including unit operations
- Feedback and feed-forward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

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

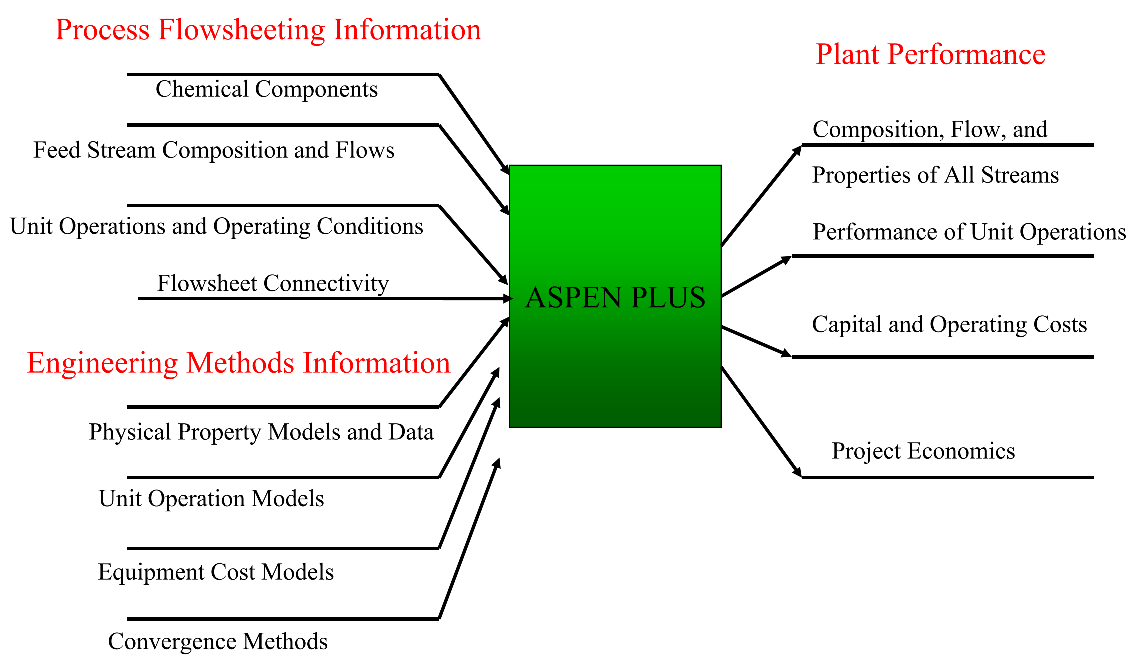
Sequential Modular Approach (SMA)

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

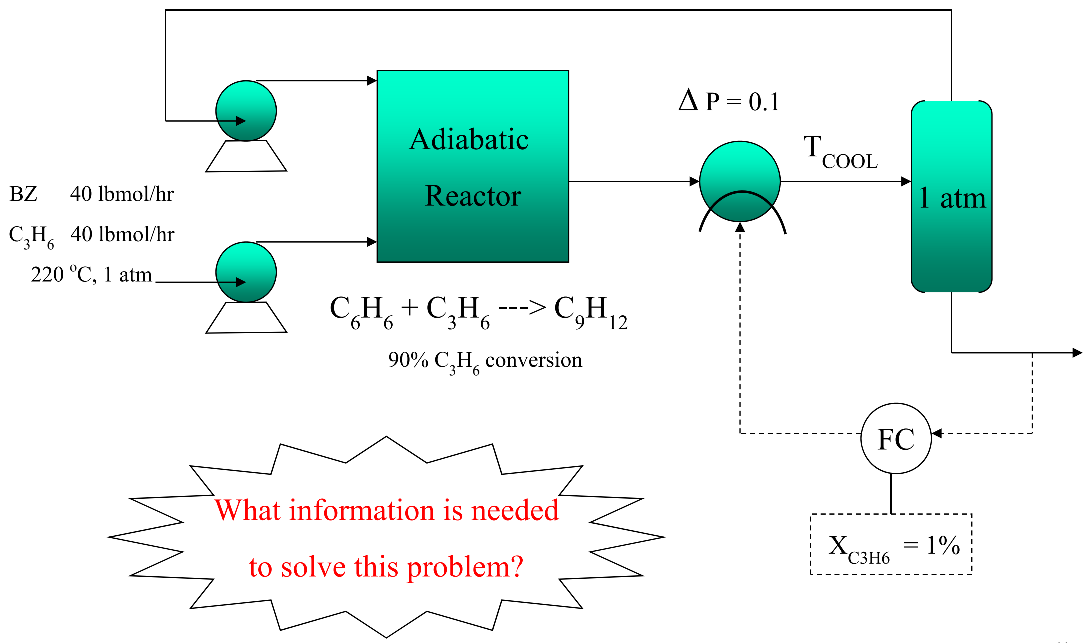


- One-block-at-a-time sequential execution: outlet stream result are used as input to the next block in the sequence

Flow of Information in a SMA Simulator



A Simulation Example Problem

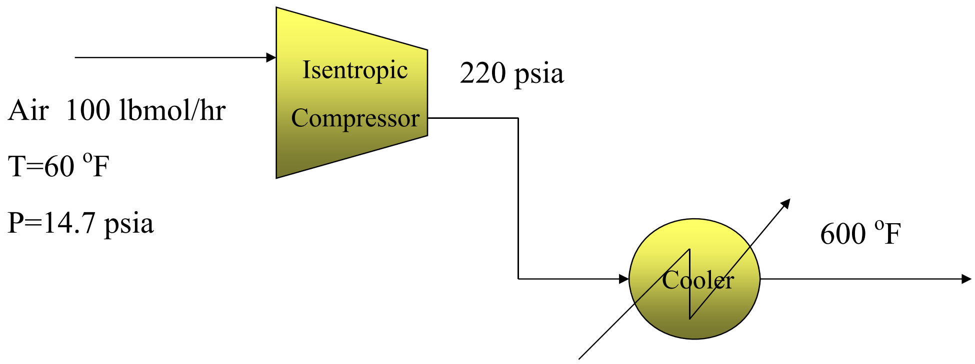


Introduction to ASPEN PLUS User Interface

- GUI consists of 2 main components

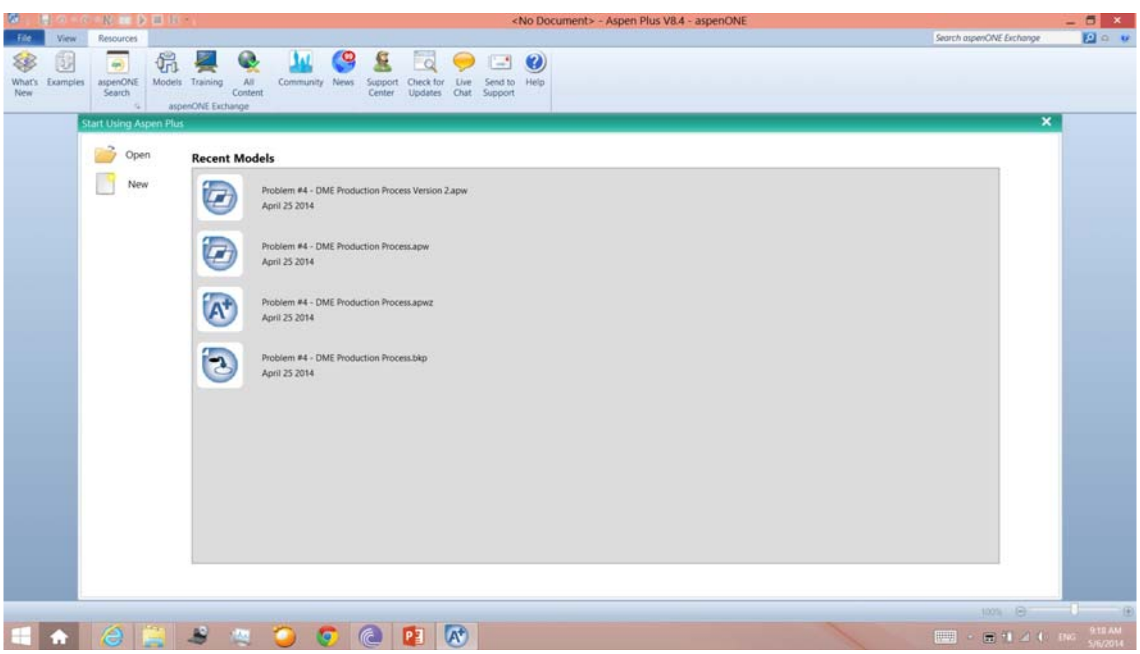
  1. Graphics
     - Flowsheet graphics
     - Results plots
     - Process flow diagrams (PFD) generation
  2. Forms and Menus
     - Help you enter process data, such as components, properties, unit operations, and other specifications to define your problem

Example Problem: Compression and Cooling of Air

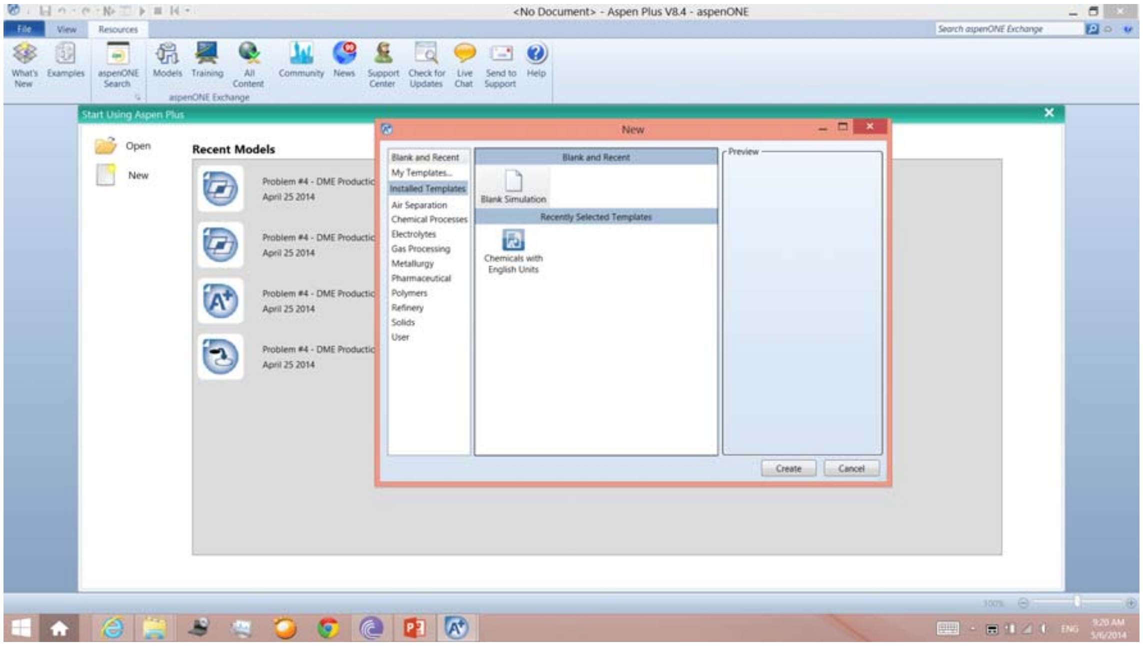


Physical property calculations: Ideal Gas vs. Redlich-Kwong-Soave

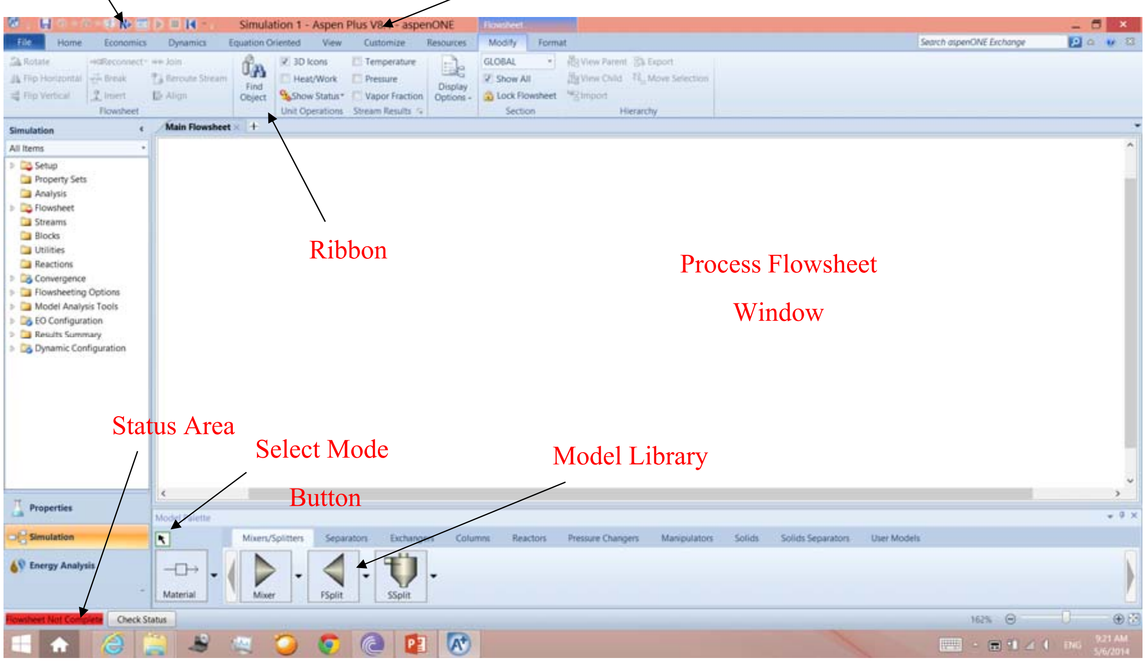
ASPEN PLUS User Interface Startup



ASPEN PLUS User Interface Startup Template



ASPEN PLUS Main Window



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:

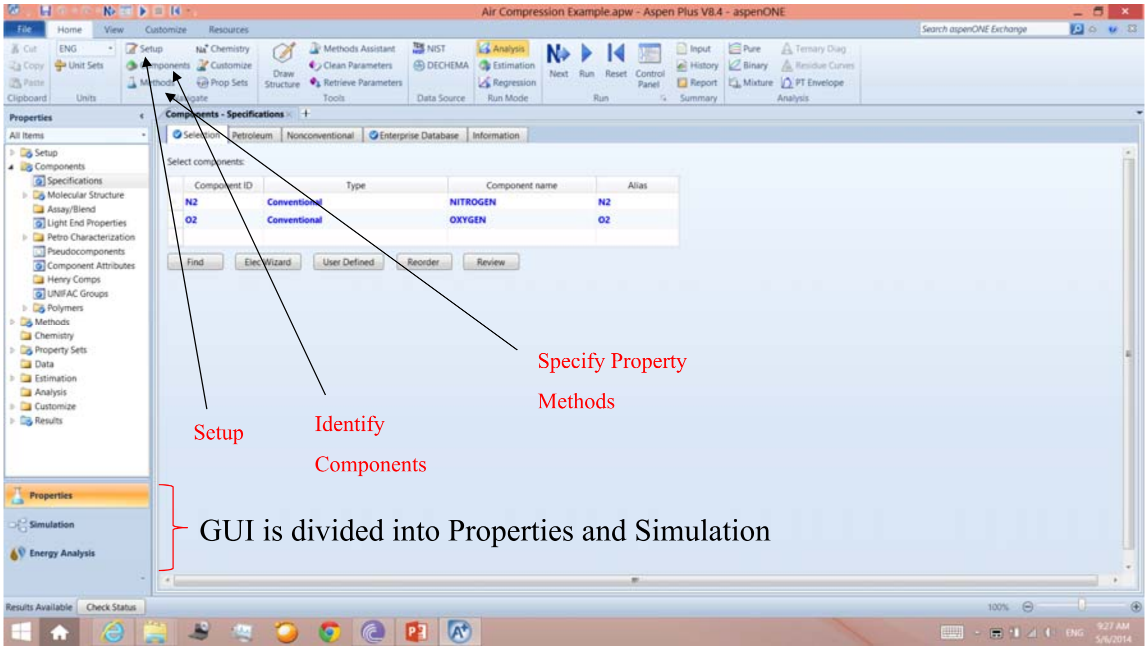
New	=> Clears workspace and starts a new run
Open	=> Opens an existing run
Save / Save As	=> Saves this run without exiting
Print	=> Prints the active window
Exit	=> Leaves ASPEN PLUS

Five Essential Elements in a Simulation Run

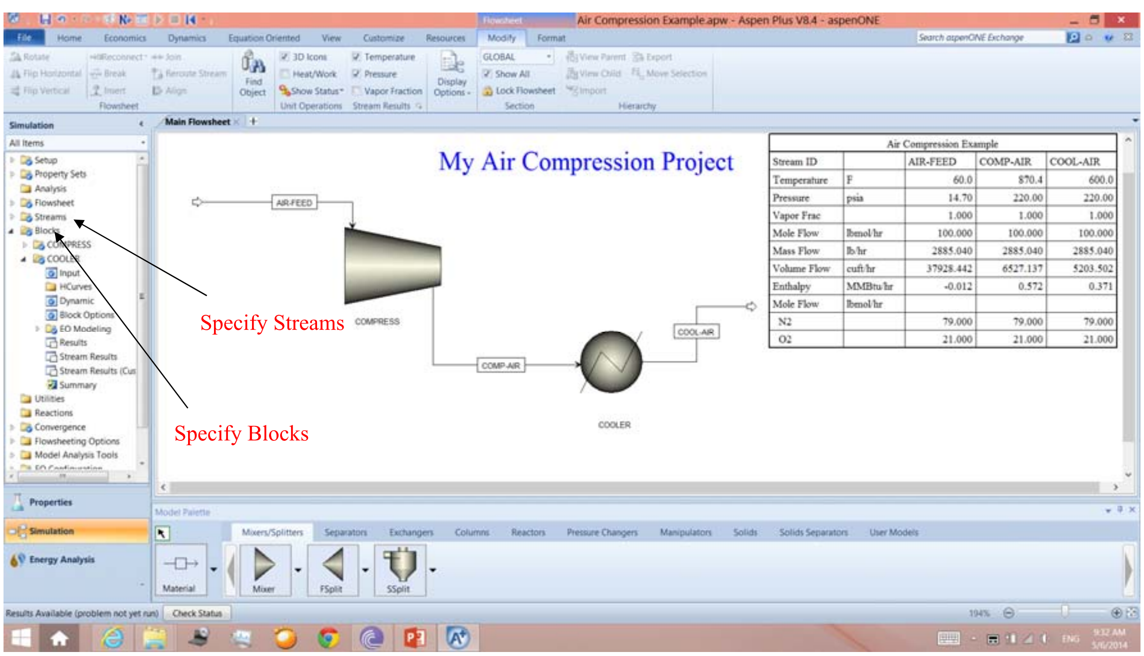
- The following 5 elements must always be specified in a simulation:

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

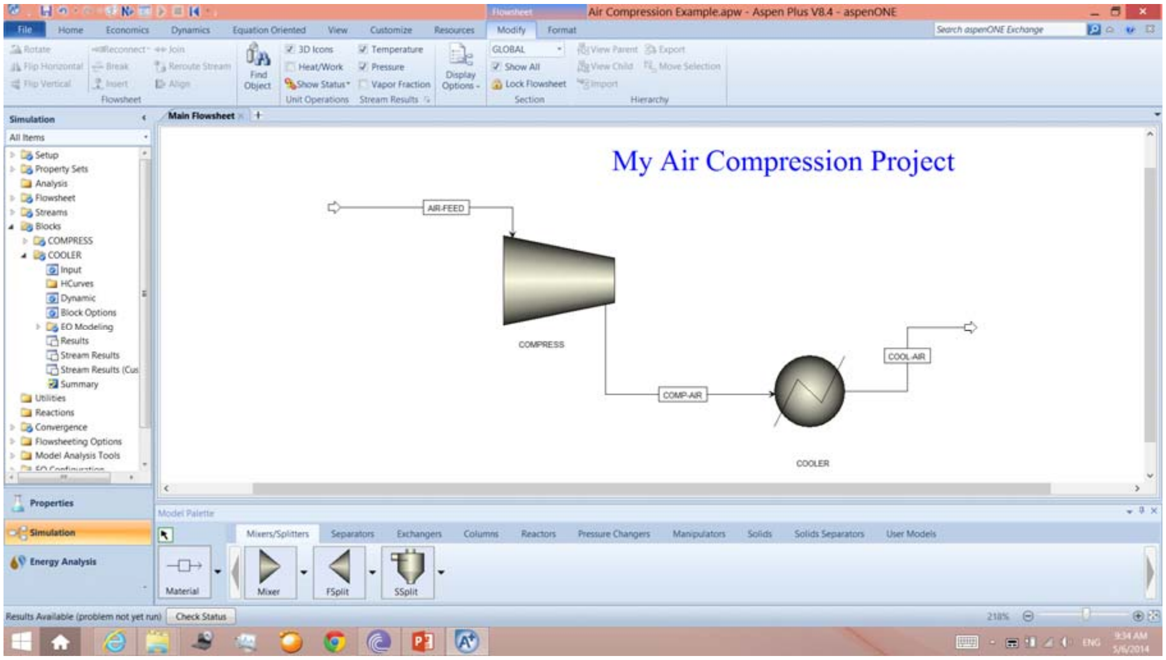
Five Essential Elements (Cont'd)



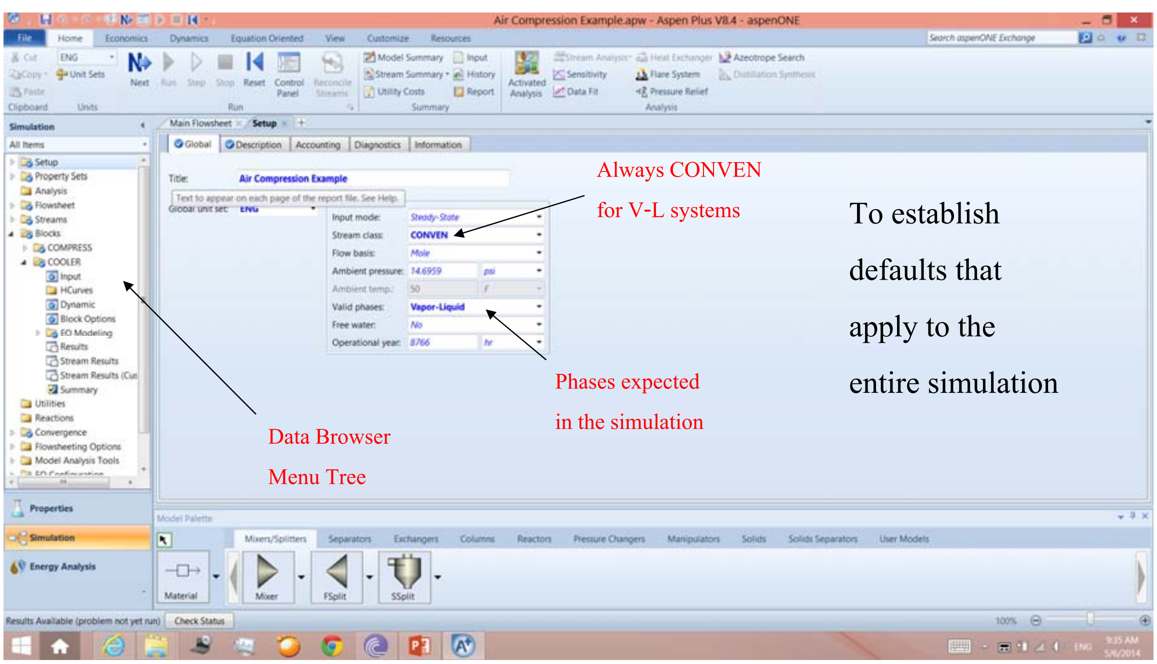
Five Essential Elements (Cont'd)



Example Problem: Compression and Cooling of Air



Air Compression Problem: Setup Sheet



Setup Sheet (Cont'd)

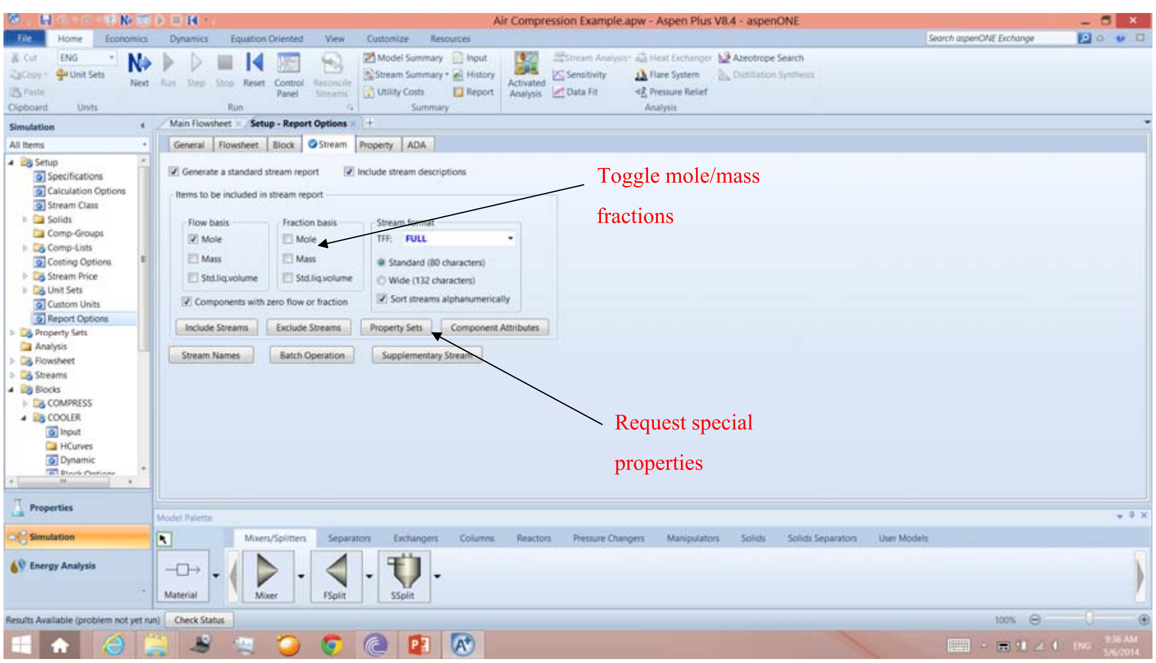
❑ Report Options

– Used to customize how simulation results and reports should look

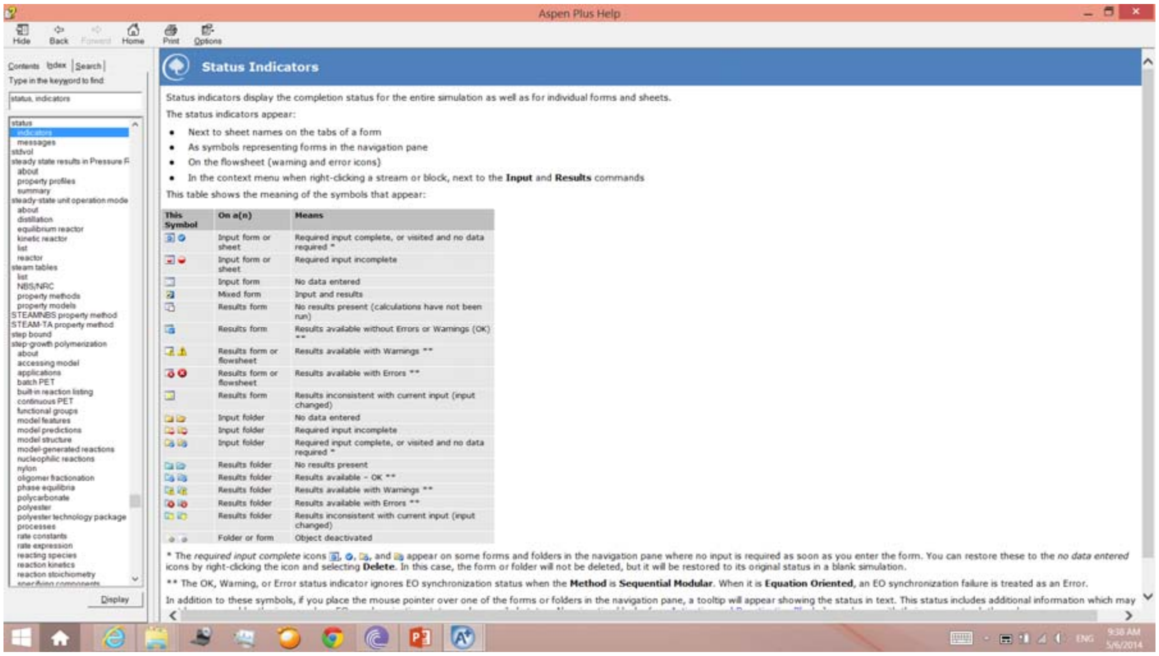
– For example, stream results can be customized to show mole fractions and mass fractions.

– Streams can also be customized to include special properties, such as viscosity, thermal conductivity, Reynolds numbers, etc.

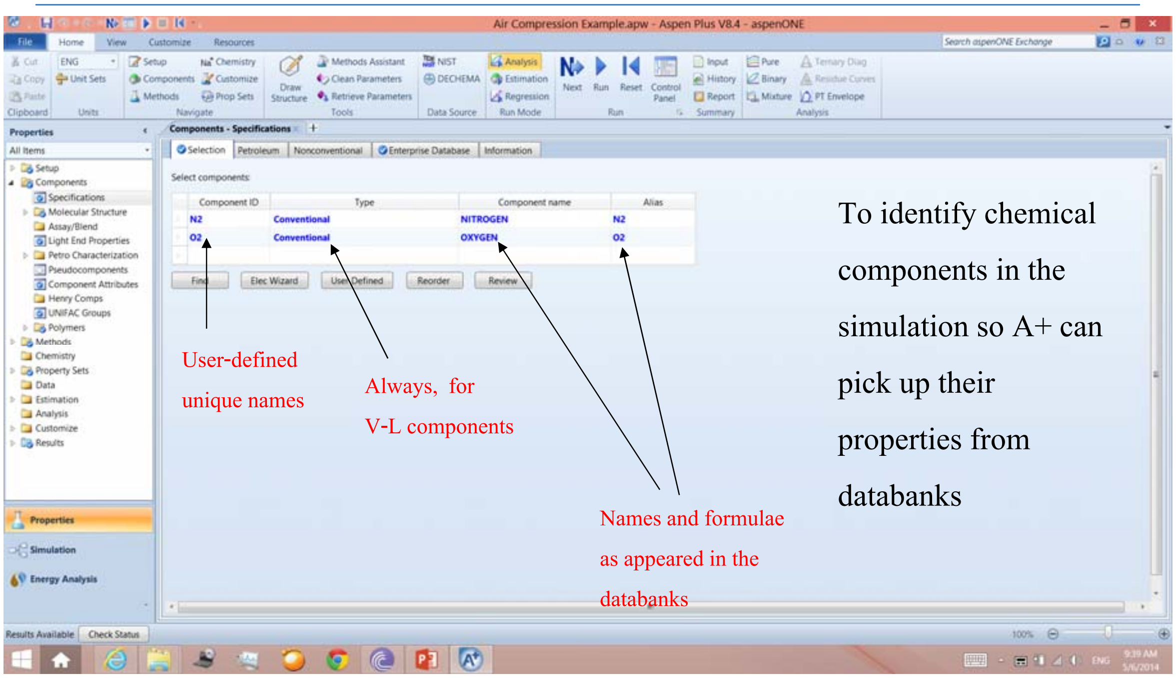
Setup Report Options Sheet for Streams



Status Indicators for Forms and Sheets



Components Specifications Sheet



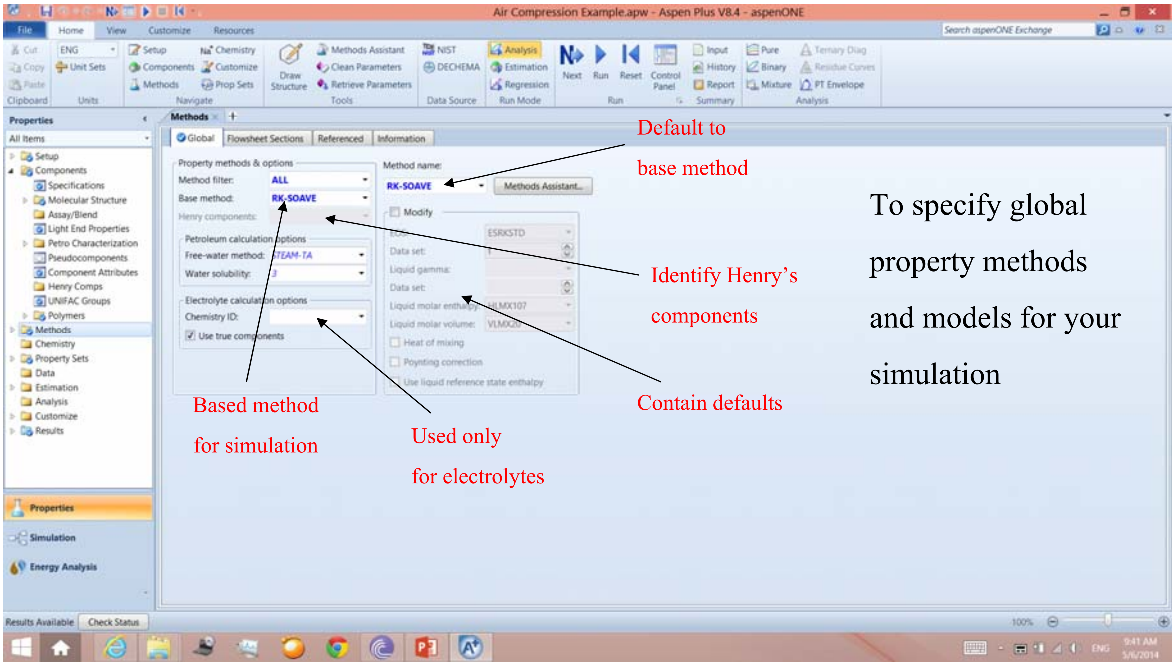
User-defined unique names

Always, for V-L components

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



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 < Vapor Fraction < 1 ---> mixed phase or two-phase stream

Feed Stream Specifications (Cont'd)

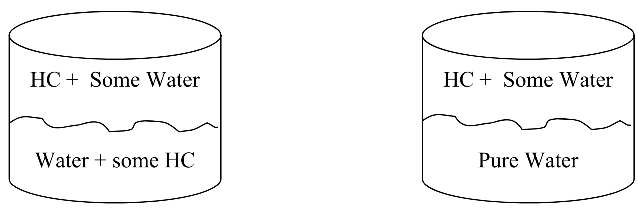
- Two options to enter feed flow rates
  1. Specify the total flow and the composition (e.g. mole fractions, mass fractions)
  2. Specify individual component flow rates.

- Several basis for Total Flow:
  - Mass, Mole, Volume, and Standard Liquid Volume (STDVOL)
  - Standard liquid volume is defined at 60 ^{o}F and 1 atmosphere

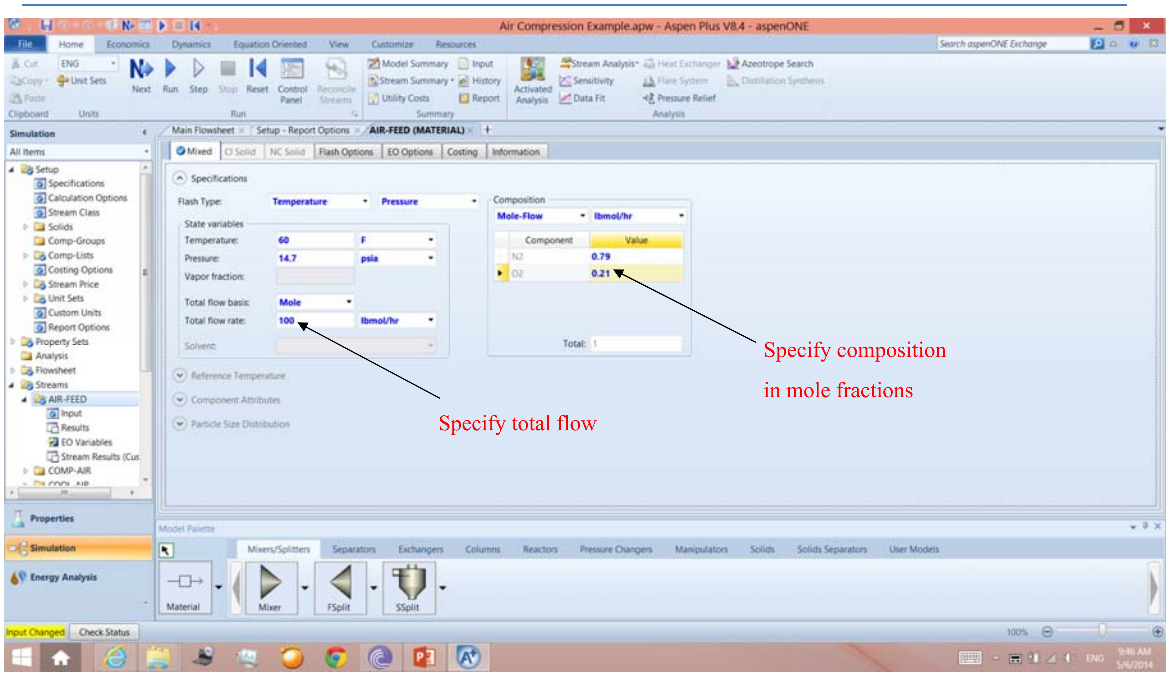
Feed Stream Specifications (Cont’d)

- 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

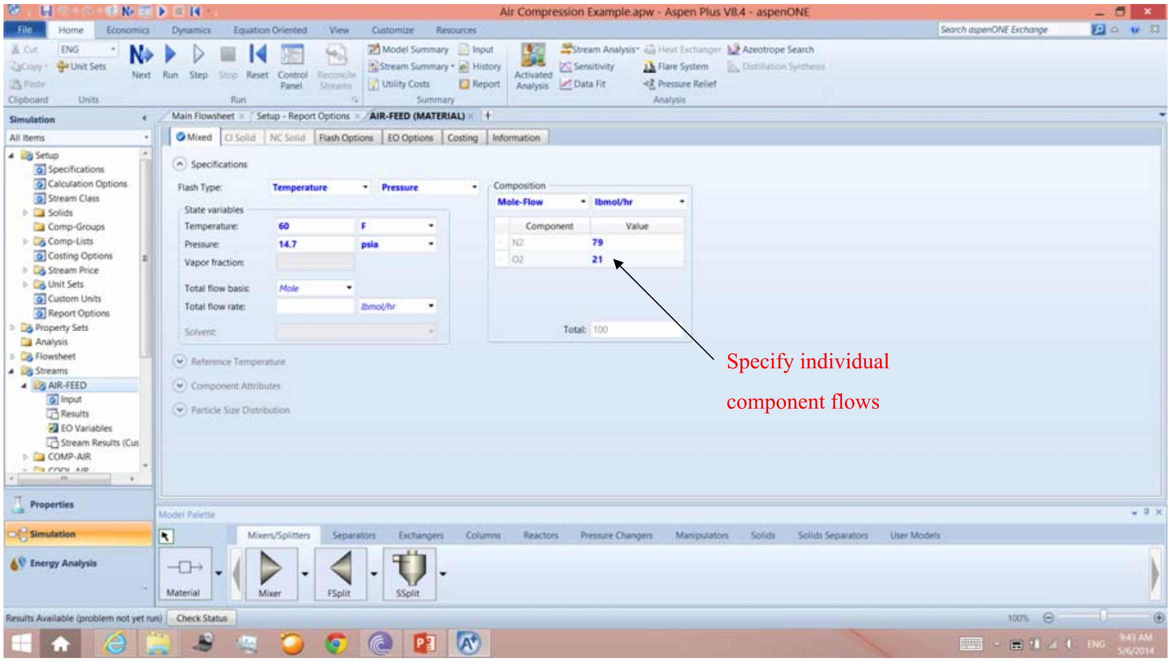
- Liquid-Liquid vs. Liquid-Freewater



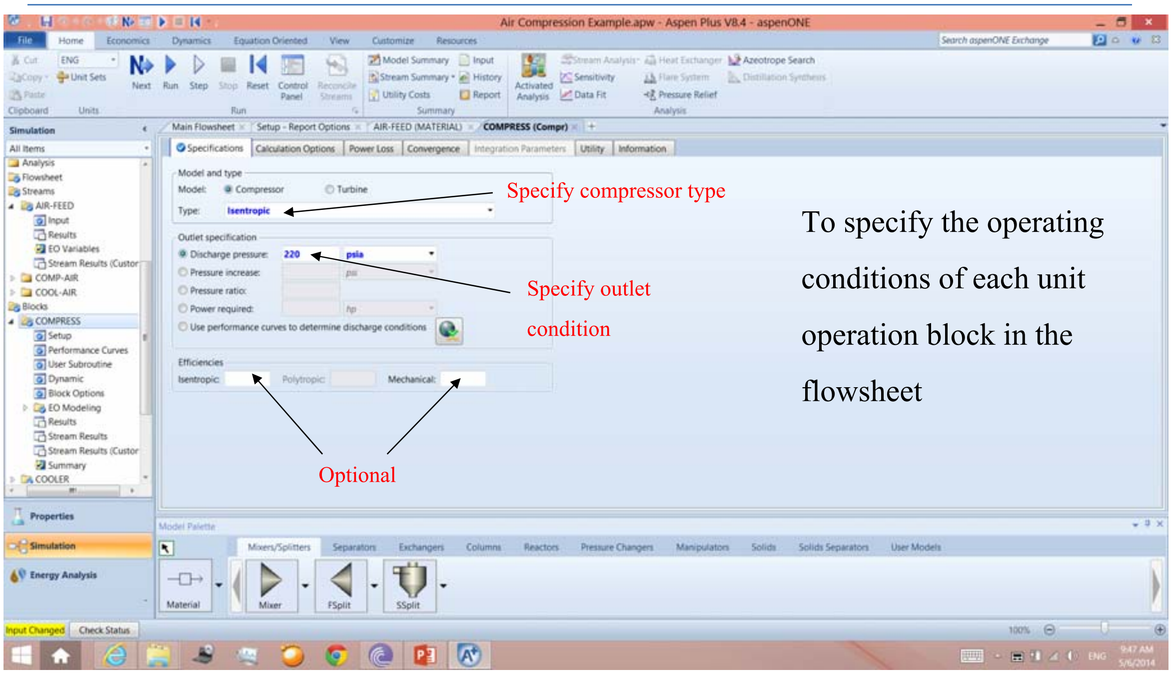
Feed Stream Specifications - Total Flow Option



Feed Stream Specifications - Component Flow Option

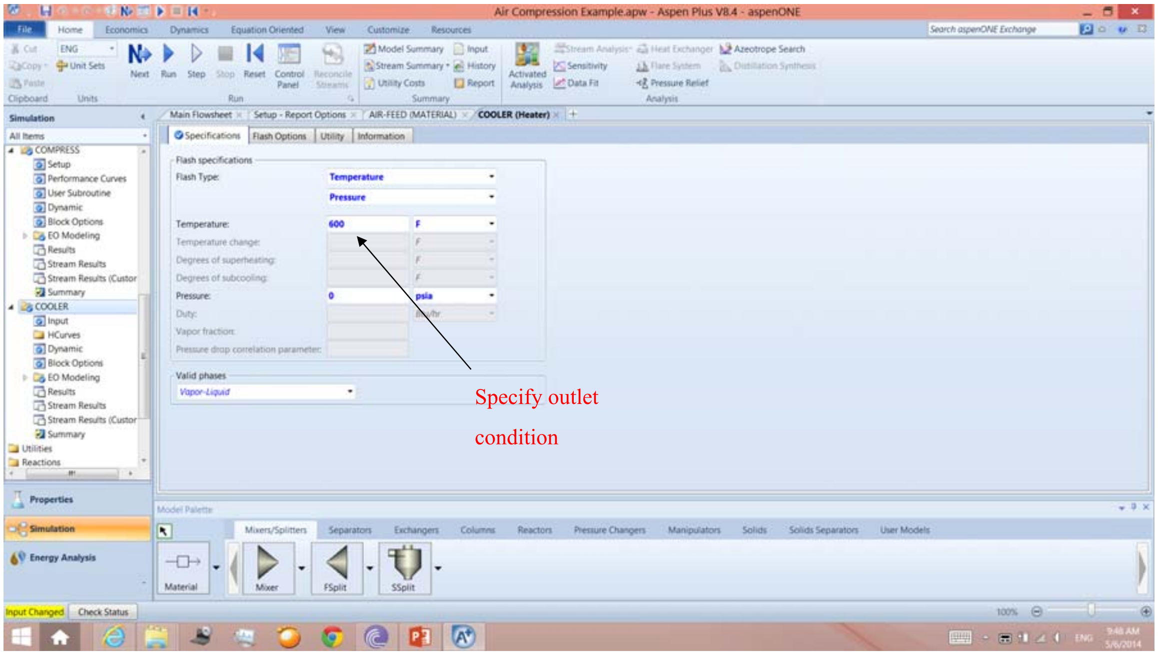


Unit Operation Block Specifications (COMPR)



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

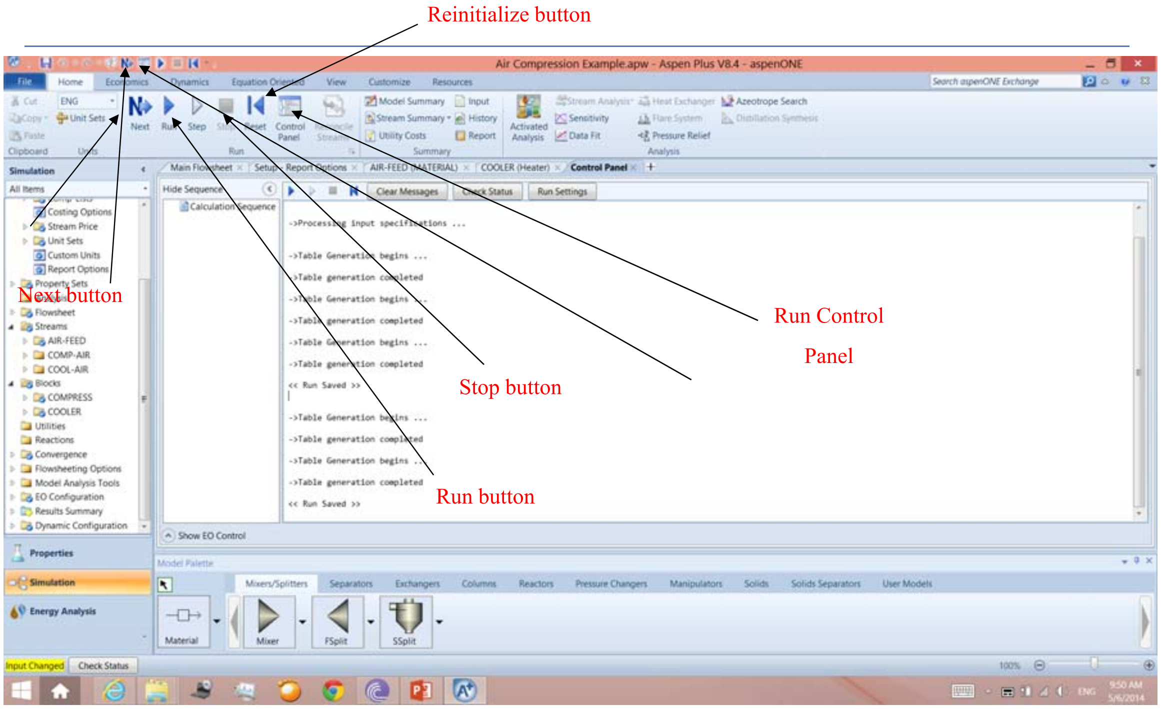
Unit Operation Block Specifications (HEATER)



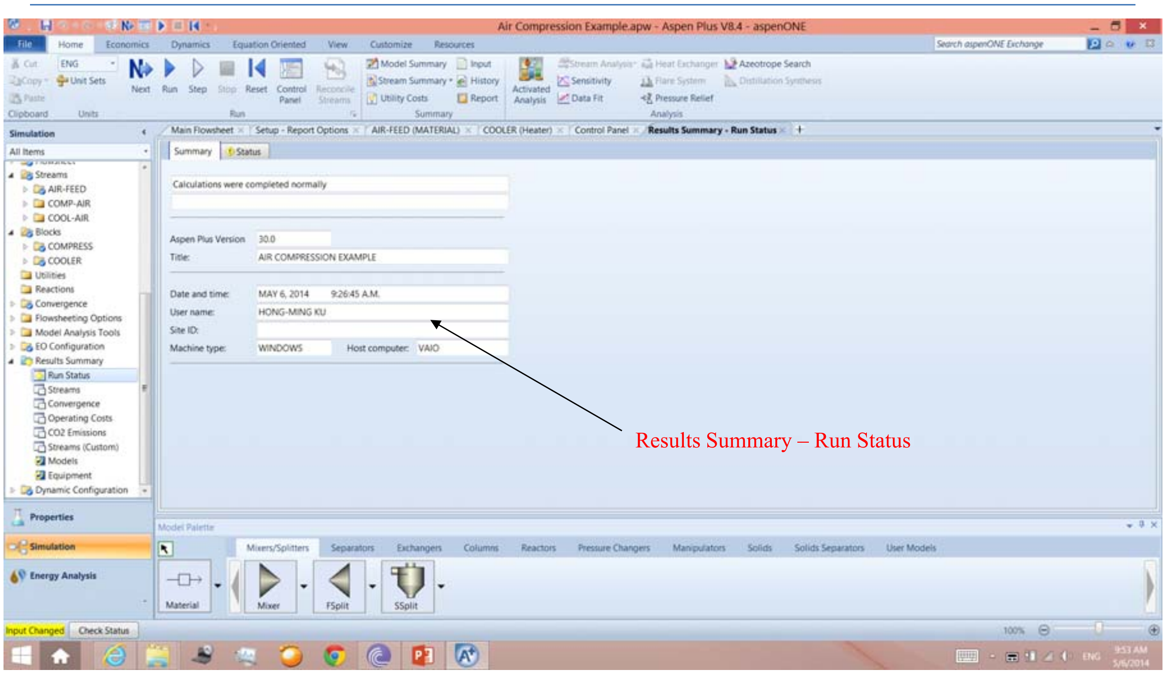
Making an ASPEN PLUS Run

- 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.

ASPEN PLUS Control Panel



Checking Simulation Results



Comparing Results: IDEAL vs. RK-SOAVE

	IDEAL Method	RK-SOAVE Method
Compressed Air Temp	870.08 ^{o} F	870.43 ^{o} 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.

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