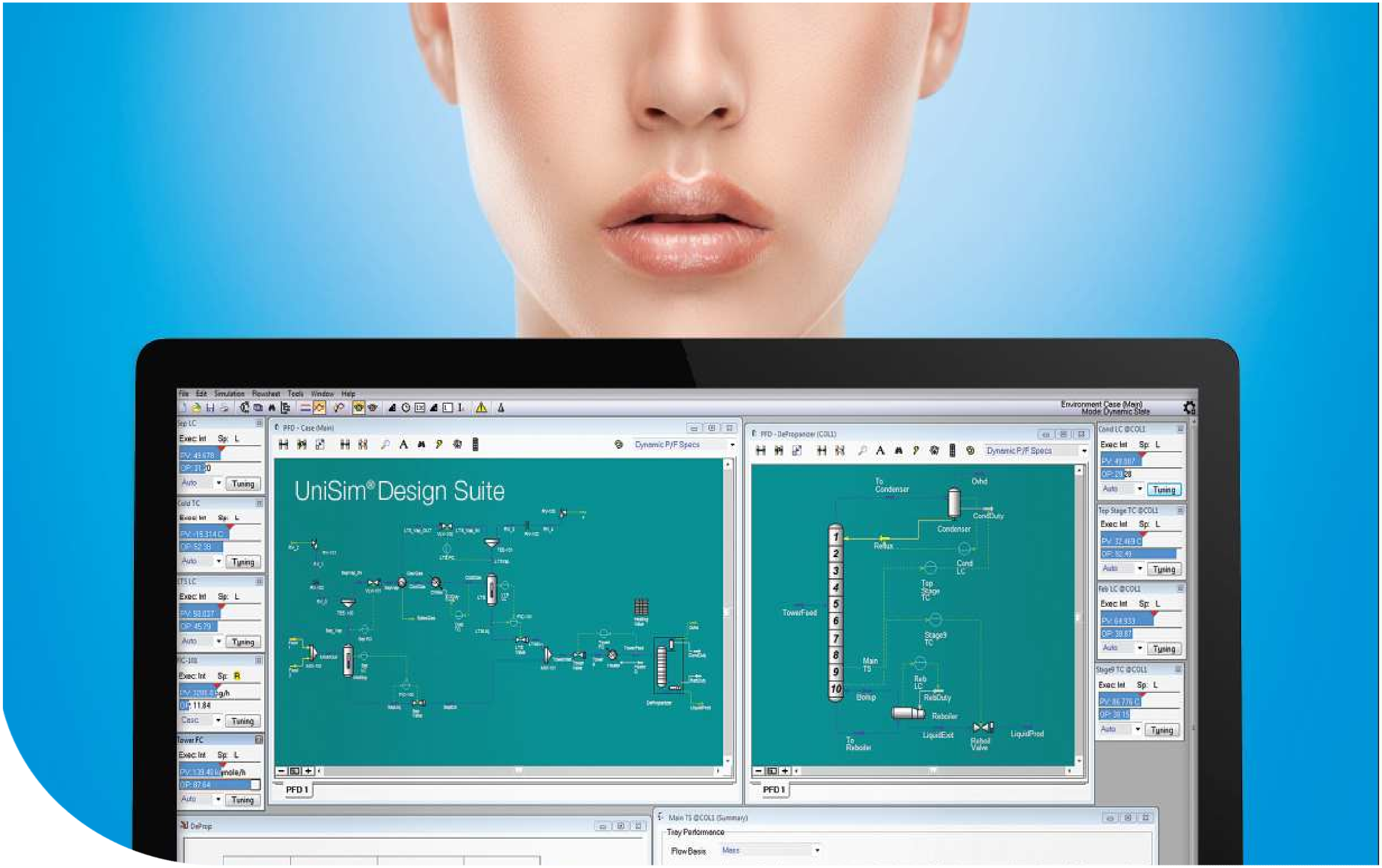


Process Modeling Fundamentals:

PDS-4526 - Process Modeling using UniSim® Design

Honeywell

Introductions

- About Me:
  - Jamie Barber
  - Chemical Engineer (BEng & PhD)
- Honeywell
  - Technical Support and Training for UniSim Design (2005-)
- AspenTech
  - Technical Support and Training for Aspen HYSYS (2002-2005)
  - Model developer for Aspen Dynamics (2000-2002)
- Based in UK

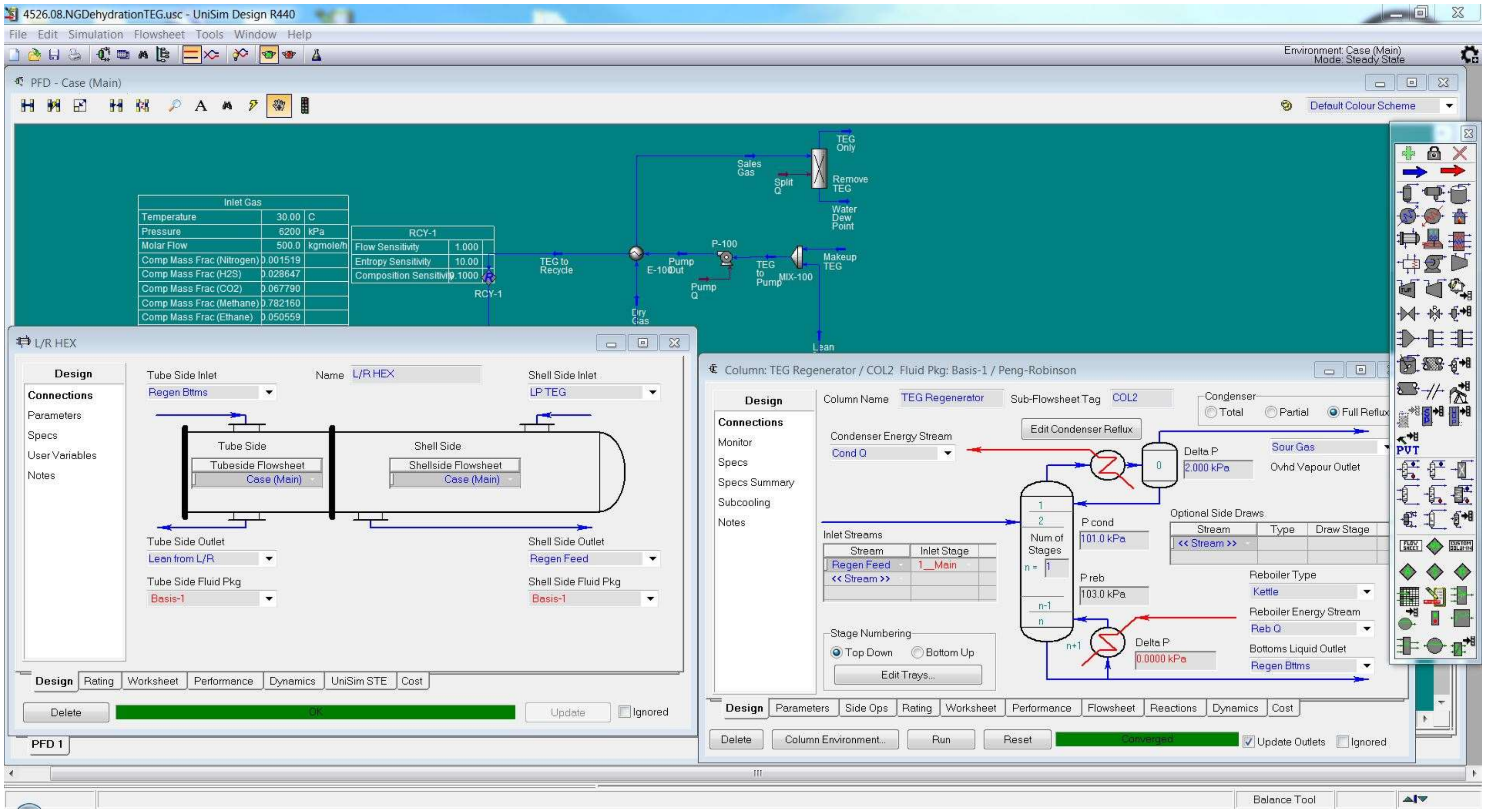
Getting Help after the course is finished

- You can contact the UniSim Design Support Team:
- Email: unisim.support@honeywell.com
- Web: honeywellprocess.com/support
- Telephone: local numbers listed on website:
  https://honeywellprocess-community.force.com/hpsservice/Search_Knowledge_Base#UniSim-Design-Suite-Contact-Us

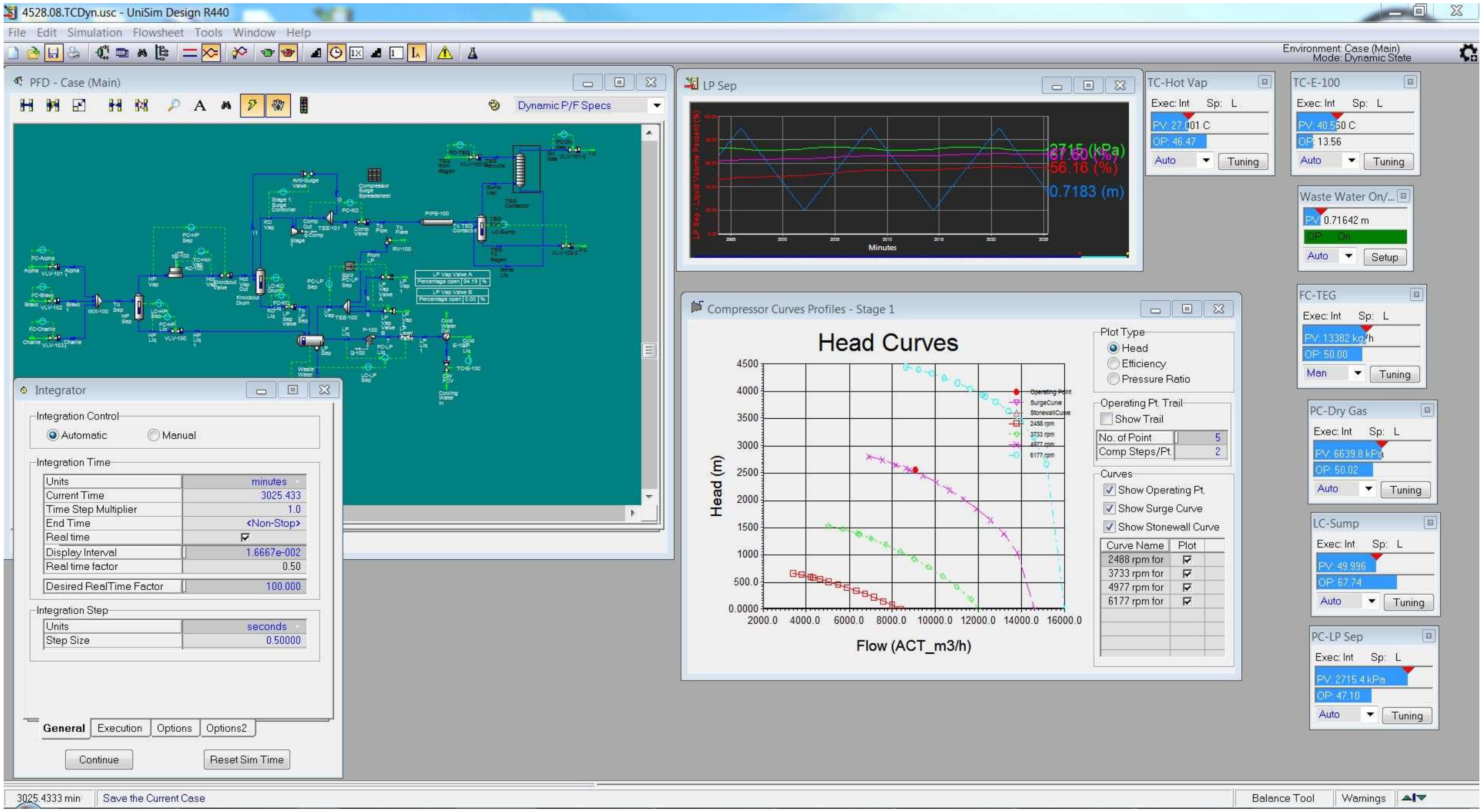
Course Outline

- Introduction to UniSim Design and UniSim Design Suite
- What is this course all about?
- Outline of the course modules
- Course modules and workshops

Process Simulation – UniSim® Design



Process Simulation – Dynamic Option



Honeywell

Course Objective

- An introduction to Steady State Modeling using UniSim® Design
- Course notes assume no knowledge of UniSim® Design

Structure of Training Material

- Material is broken into several modules (chapters)
- Each module will focus on one or more areas
- Most of your time will be spent working on your own. This type of "Hands on" training is very effective.

"Tell me and I forget,
Show me and I may remember,
Involve me and I understand."

Benjamin Franklin
Scientist, Statesman

Outline of Modules

- Module 1 – Getting Started
  - Introduction to the UniSim Design interface.
- Module 2 – Propane Refrigeration Loop
  - Build a simple flowsheet with 4 streams and 4 operations.
- Module 3 – Refrigerated Gas Plant
  - Build a more complex flowsheet, use logical operations.
- Module 4 – NGL Fractionation Train
  - Build a distillation train with 3 columns in series.
- Module 5 – Oil Characterization
  - Use the UniSim Design Oil Manager to characterize an oil.

Outline of Modules – Day 2

- Module 6 – Two Stage Compression
  - Create a model of a two stage compressor train. Use the recycle operation for the first time.
  - Use the pipe segment and the Simulation Balance Tool.
- Module 7 – Acid Gas Sweetening with DEA
  - Create a flowsheet to model the removal of H2S and CO2 from a sour gas. Use the Amine package in UniSim Design.
- Module 8 – Natural Gas Dehydration with TEG
  - Create a flowsheet to model the removal of water from a natural gas stream with TEG.
- Module 9 – Reporting with UniSim
  - A quick look at the different options for generating data with UniSim Design.

Honeywell

Module 1 – Getting Started

- Introduction to the UniSim Design interface.

- In the Basis Environment, you will…
  - Select an appropriate property package
  - Create a component list
  - Export the Fluid Package (Prop. Pkg and Comp. List) for use later.

- In the Simulation Environment, you will…
  - Create streams
  - Perform stream analysis
  - Work with stream flash calculations
  - Attach stream utilities
  - Customize the workbook

Process Simulation

- What information do we need to enter?

- Thermodynamic Information
  - A list of all the components that are needed.
  - Selection of an appropriate model.
    - Could be an EOS (PR or SRK) or an Activity Model (NRTL or UNIQUAC)

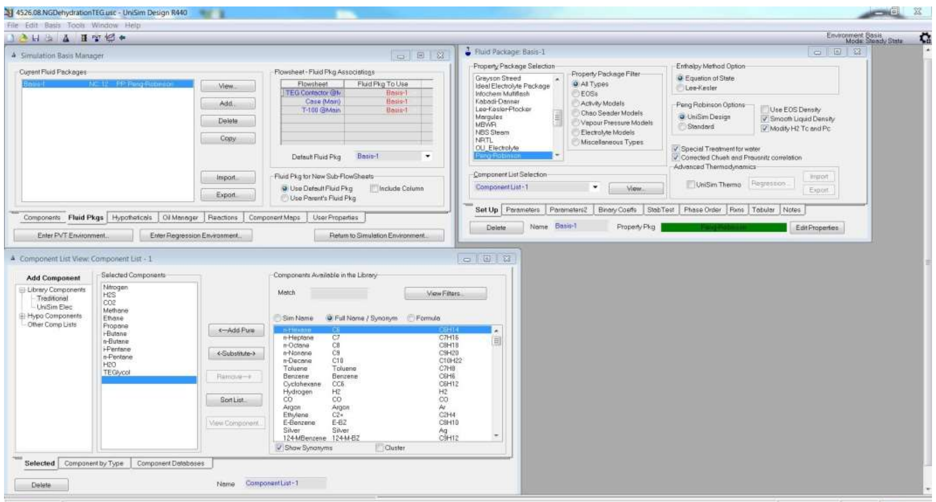
- Process Information
  - Feed stream conditions. (T, P, Flow, Composition)
  - Unit operation information.
  - What unit operations are needed?

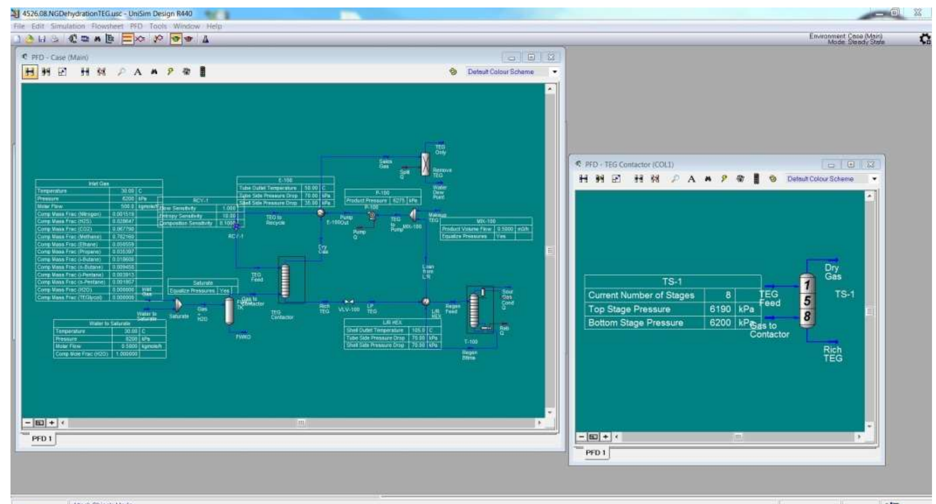
How do we do this in UniSim Design?

- Via the two main USD Environments

Basis Environment

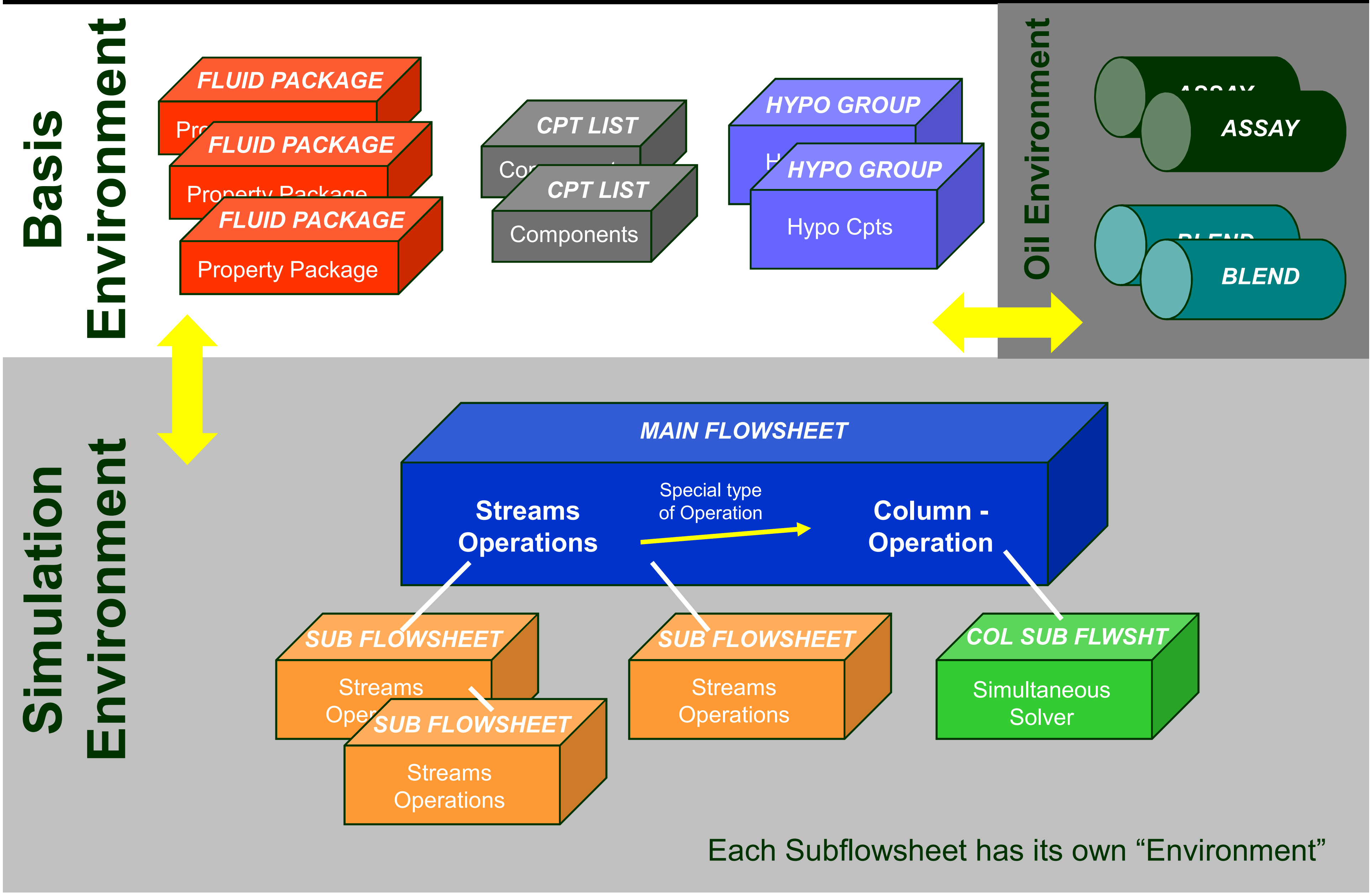
Simulation Environment





Honeywell

UniSim Design Architecture



Basis Environment

- Every Fluid Package needs a component list and a property package.
- The Peng-Robinson EOS has been optimized for use with most Oil & Gas applications in UniSim Design.
- It is very important the right property package is chosen. The accuracy of the model depends on this choice.
- The “Master” component list is a superset of all components in the other lists. It cannot be selected as the component list for use in a fluid package.
- Fluid Packages can be exported and shared with colleagues.

Honeywell

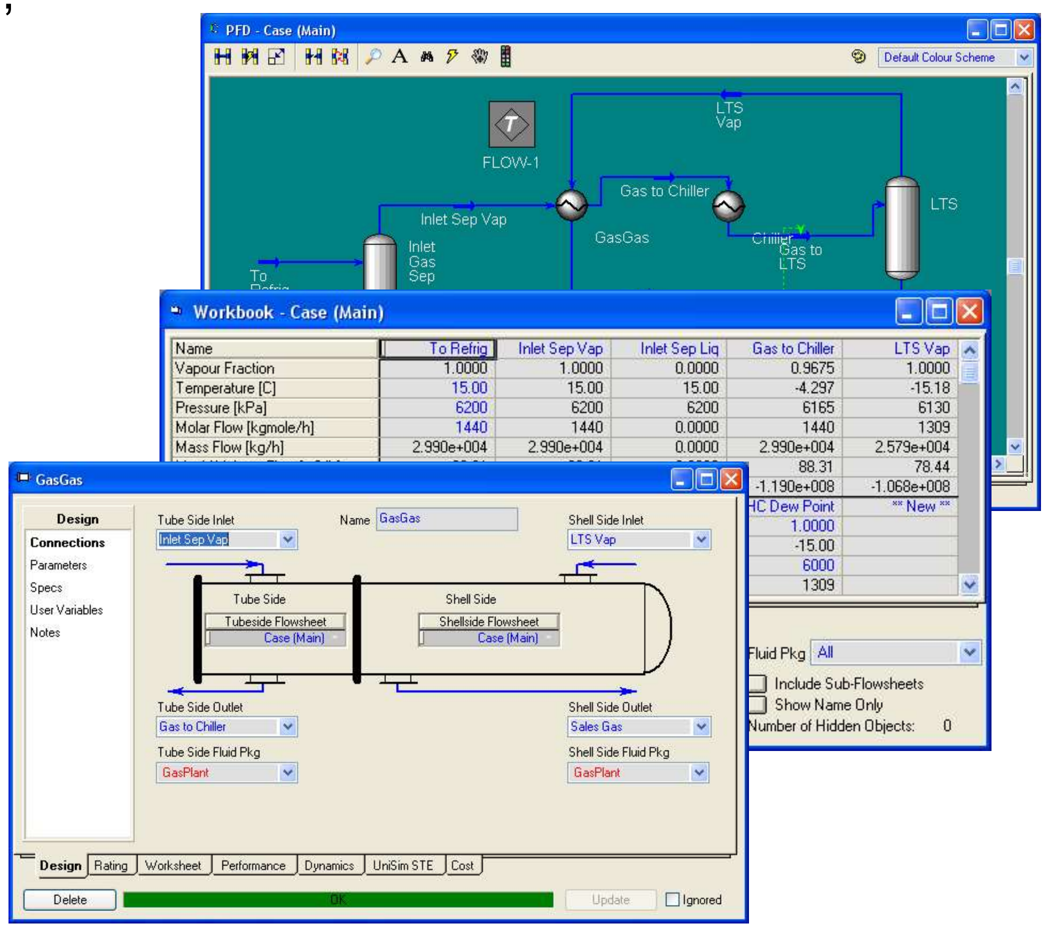
Preferred UniSim Property Package

Type of System	Recommended Property Method
TEG Dehydration	PR
Sour Water	Sour PR
Cryogenic Gas Processing	PR, PRSV
Air Separation	PR, PRSV
Atm Crude Towers	PR, PR Options, GS
Vacuum Towers	PR, PR Options, GS(<10mmHg), Braun K10, Esso K
Ethylene Towers	Lee Kesler Plocker
High H2 Systems	PR, ZJ or GS (see T/P limits)
Reservoir Systems	PR, PR Options
Steam Systems	Steam Package, CS or GS
Hydrate Inhibition	PR
Chemical Systems	Activity Models, PRSV
HF Alkylation	PRSV, NRTL
TEG Dehydration with Aromatics	PR

Simulation Environment

- Key Features
  - Calculates Bi-Directionally
  - Calculates as much as it can, as soon as it can

- Primary Interface Elements
  - PFD
  - Workbook
  - Object Property Views



Honeywell

Tips for adding streams and operations

- There are four methods for adding objects
  - Flowsheet Menu, F11, Object Palette, Workbook

- [Unit Operations are added similarly]

- Streams can also be added by typing their name into the connections page for a unit operation.
  - Use this option carefully as a simple typo will result in a undesired result.

Stream Calculations

- Intensive Calculations
  - Flash (Phase Equilibrium) & Property Calculations
  - "Stream" Utilities – Phase Envelope, Property Table, Hydrate Formation, CO_2 Freeze Out, BP Curves, etc.

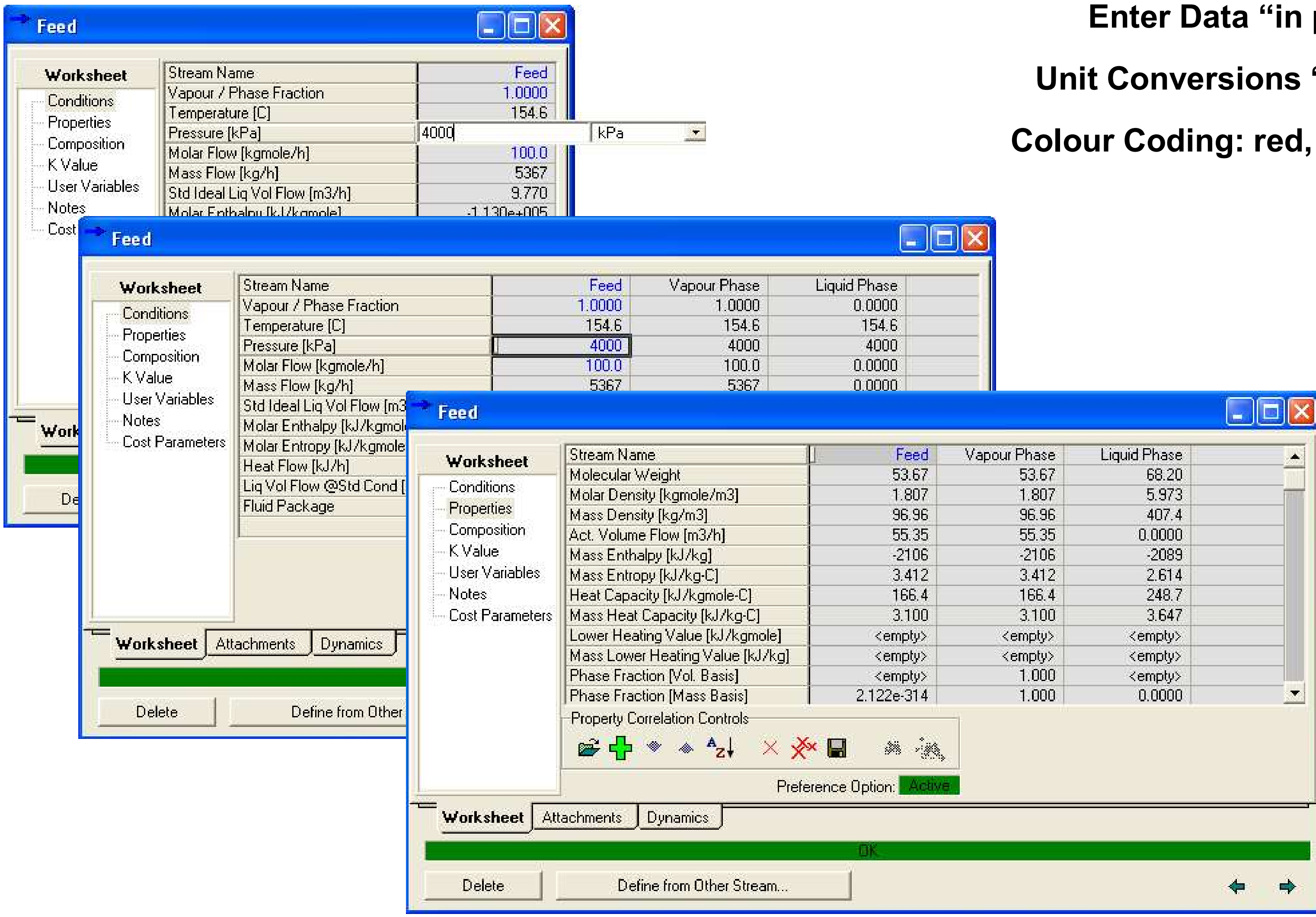
- Extensive Calculations (required for flowsheeting)
  - Material Flows
  - Energy Flows

Honeywell

Degrees of Freedom in UniSim Design

- For streams, only two of the five “state” variables can be specified. (P, T, H, S, or VF).
- Normally, the user will specify T-P, T-VF, or P-VF.
- For dew point calculations, Set the VF = 1, and enter T or P. UniSim Design will calculate the other parameters based on the thermo model that has been chosen.
- Likewise, the bubble point can be found by setting the VF to 0.
- Never specify more than one type of flow.
  - Mole, Mass, Liquid Volume @ std. cond. or Std. Ideal Liquid Volume

Stream Property View – Input & Output



Enter Data "in place"

Unit Conversions "in place"

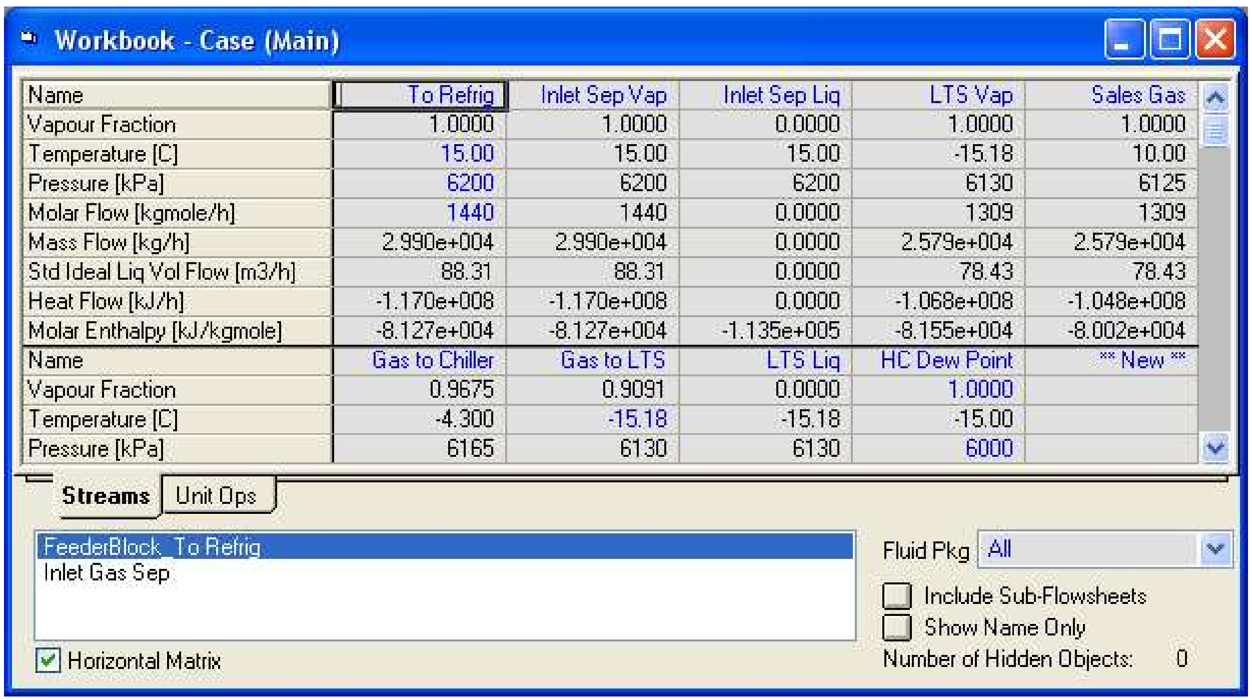
Colour Coding: red, blue, black

Honeywell

Tips – Using the Workbook

- Useful to create custom PFD tables, stream reports, copy/paste stream data, troubleshooting flowsheets, changing stream data

- Set up once; then export for future usage



Name	To Refrig	Inlet Sep Vap	Inlet Sep Liq	LTS Vap	Sales Gas
Vapour Fraction	1.0000	1.0000	0.0000	1.0000	1.0000
Temperature [C]	15.00	15.00	15.00	-15.18	10.00
Pressure [kPa]	6200	6200	6200	6130	6125
Molar Flow [kgmole/h]	1440	1440	0.0000	1309	1309
Mass Flow [kg/h]	2.990e+004	2.990e+004	0.0000	2.579e+004	2.579e+004
Std Ideal Liq Vol Flow [m3/h]	88.31	88.31	0.0000	78.43	78.43
Heat Flow [kJ/h]	-1.170e+008	-1.170e+008	0.0000	-1.068e+008	-1.048e+008
Molar Enthalpy [kJ/kgmole]	-8.127e+004	-8.127e+004	-1.135e+005	-8.155e+004	-8.002e+004
Name	Gas to Chiller	Gas to LTS	LTS Liq	HC Dew Point	** New **
Vapour Fraction	0.9675	0.9091	0.0000	1.0000	
Temperature [C]	-4.300	-15.18	-15.18	-15.00	
Pressure [kPa]	6165	6130	6130	6000	

Honeywell

Utilities in UniSim Design

- There are two main types of Utilities in UniSim Design:
  - Stream Utilities
  - Operation Utilities

- Stream utilities are attached to streams and include items like: envelopes, property tables, hydrate, etc.

- Operation utilities are attached to operations and include: tray sizing, vessel sizing, and pipe sizing.

- There are other utilities that do not attach to either streams or operations. These include the property balance utility and the optimization utilities.

Module 2 – Propane Refrigeration Loop

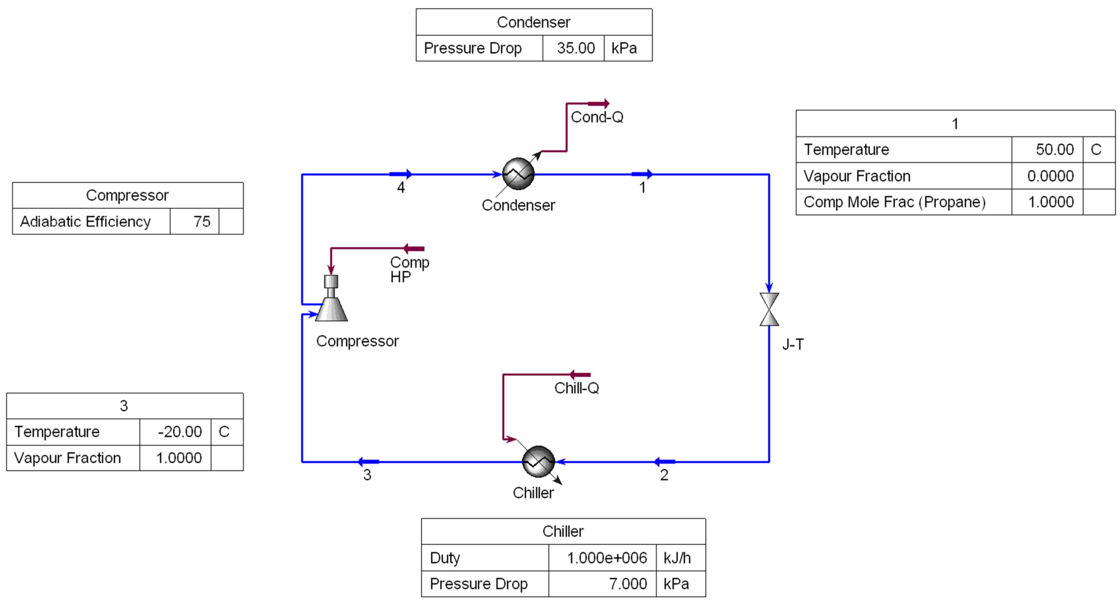
- Objectives
  - Build a simple flowsheet in UniSim Design
  - Understand and investigate the forward/backward flow of information in UniSim Design
  - Use the graphical interface to display information
  - Convert the simulation case into a template for future use

- Unit Operations that are covered
  - Heater
  - Cooler
  - Valve
  - Compressor

Honeywell

Module 2 – The Process

- Circulate Propane through a cooler where it is condensed, a valve to lower the pressure, a 'chiller' where it is vaporized, and then recompress it in a compressor.
- Heat enters the loop in the 'chiller' and leaves in the cooler.



Honeywell

Placing Objects on the Flowsheet

- Use the PFD Object Palette, Flowsheet Menu, F11(streams)/F12(operations), or Workbook

- Objects are given default names unless the user specifies a name
  - The default naming scheme can be set by the user in the Simulation Preferences

- There are multiple methods to connect streams and unit operations:
  - Drop down boxes (e.g. type a new name in box for NEW streams)
  - Attach & Auto-Attach modes


Using the Mouse Buttons

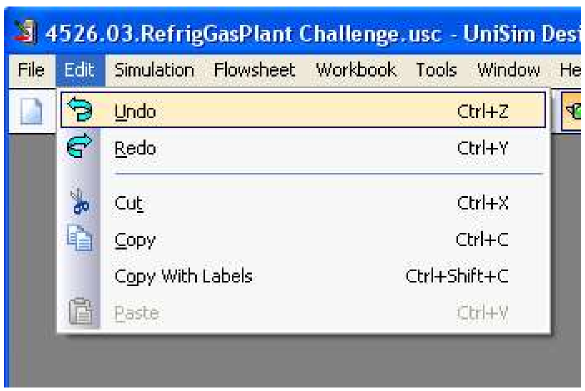
- Left click - Select… object or item
- Left click & drag - Move the object
  - Select multiple objects by drawing a box around them
- Right click - Object-inspect menu
- Right click & drag - Drag and drop (bull’s eye)

Tips for working with the PFD

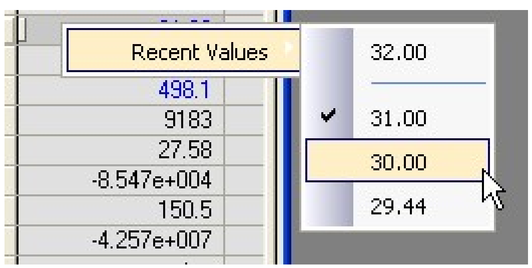
- Know the Hot Key options (Shift+T, P, F, M & N)
- Right-click on any object to bring up the “Object Inspection” menu
- Hover cursor over a stream to bring up the “Tool Tip”
- Add Tables to streams and operations to see key data on the PFD
- Hiding items can create a cleaner view; however, it can make it harder to debug a model.

Undo / Redo / Recent Values

- Undo also supported for PFD moves and icon resizes
  - Not for object deletions
- Stores unlimited history of changes in object windows
  - Memory is wiped when the window is closed



From Edit menu or [or CTRL+Z, CTRL+Y]



Access Recent Values option by right clicking on a value

Honeywell

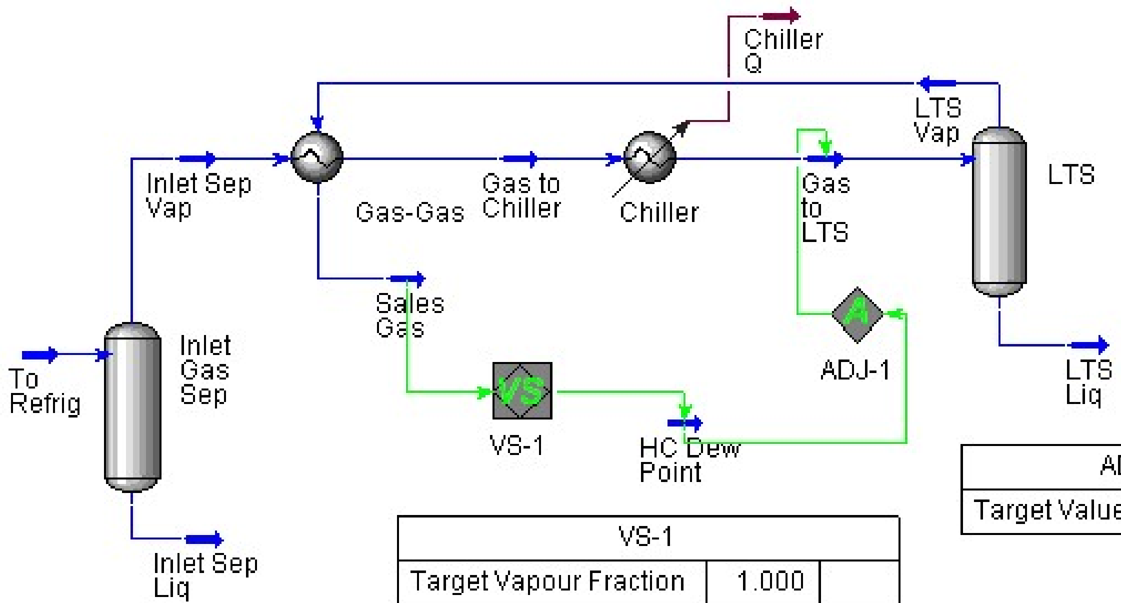
Sub-flowsheets and Templates

- The Main Flowsheet in UniSim Design can contain several sub-flowsheets.
- Each sub-flowsheet can have its own fluid package.
- Templates are ‘pre-built’ sub-flowsheets that are saved as UTPL files. They are useful for creating reusable models sections that could be used in several different cases.

Module 3 – Refrigerated Gas Plant

- Objectives:
  - Install and use the Heat Exchanger operation
  - Use logical operations (Virtual Stream and Adjust)
  - Use the Case Study tool to study the behavior of the model

Module 3 – The Process



ADJ-1		
Target Value	-15.00	C

VS-1		
Target Vapour Fraction	1.000	
Target Temperature	-15.00	C
Target Pressure	6000	kPa

Introduction to Heat Exchanger Calculations

- The Heat Balance must be satisfied:

$$(Q_{COLD} - Q_{leak}) - (Q_{HOT} - Q_{loss}) = 0$$

$$Q_{COLD} = M_{COLD} {}^{*}\Delta H_{COLD}$$

$$Q_{HOT} = M_{HOT} {}^{*}\Delta H_{HOT}$$

Can be solved for T, H, Mass/Mole Flow, or UA.

$$LMTD = (\Delta T_1 - \Delta T_2)/\ln(\Delta T_1/\Delta T_2)$$

$$\Delta T_1 = T_{hot,in} - T_{cold,out}$$

$$\Delta T_2 = T_{hot,out} - T_{cold,in}$$

Heat Exchanger Specifications

- Heat Balance = 0
  - This is the default spec and can not be changed or made inactive.
- Temperature
- Minimum Approach
  - Closest temperature between hot and cold passes
- Overall UA or LMTD
  - For no phase change, the end point model is OK
  - For phase change, the weighted model is best
- Pressure Drops
  - Usually specified with simple models, can be calculated with rating models.

Introduction to the Virtual Stream Operation

- Provides a general purpose facility to create a live copy of the data from one stream (the Reference stream) to another (the Target stream).

- To make a duplicate of a stream, four reference variables must be selected:
  - Composition must be selected
  - Flow (molar or mass)
  - Two others of either: Vapour Fraction, Temperature, Pressure, and Enthalpy

- The Virtual Stream operation may also be used to perform flash calculations – Composition must be selected as the first variable.

- The Virtual Stream operation shows green connections because it does not imply a material balance.

Tips on the Adjust Operation

- How it works – Adjusts the independent variable until the dependant variable meets the target value within the set tolerance.

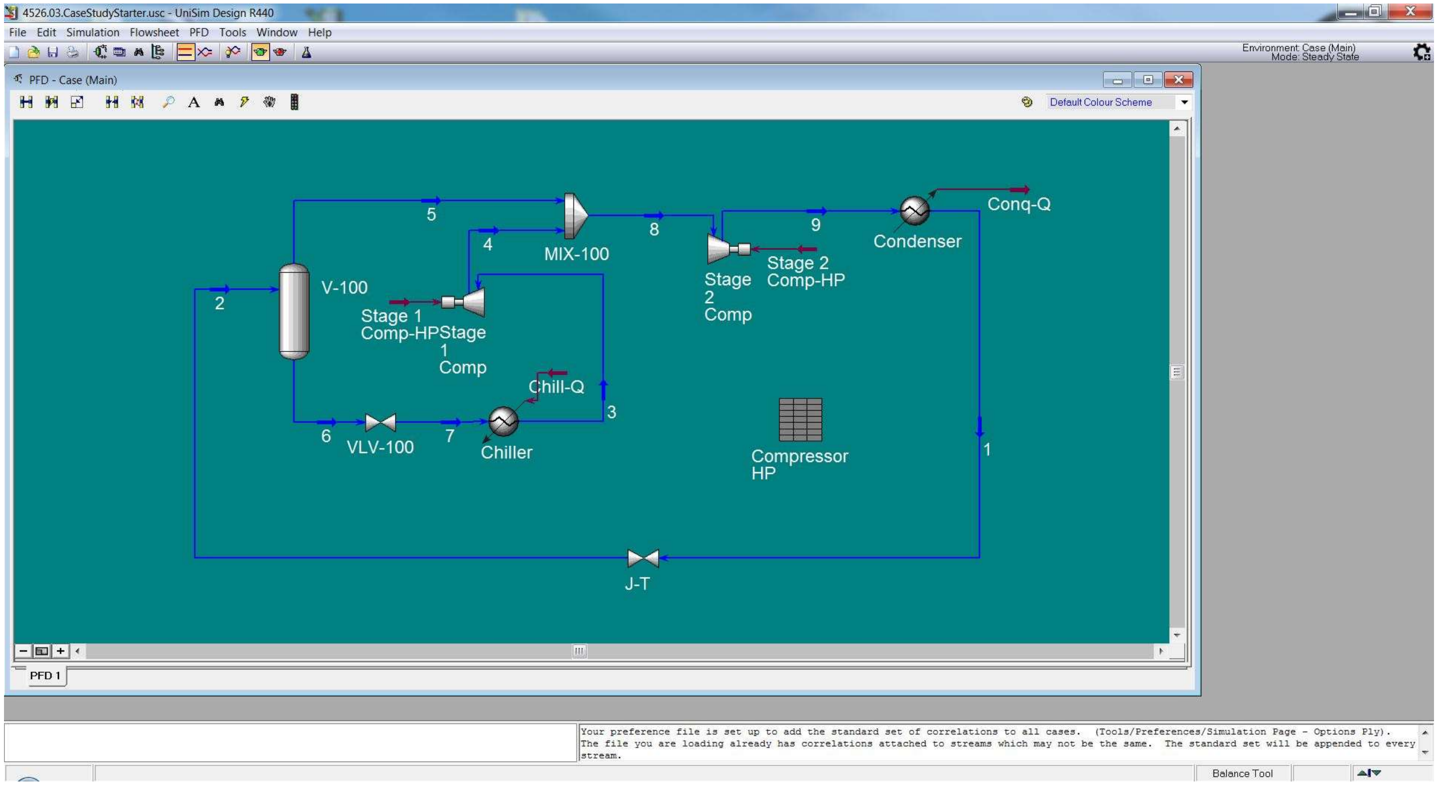
- Some Tips:
  - Solve the flowsheet first.
  - The variable that will be adjusted (independent variable) must be a blue value. (it must be user modifiable.)
  - A good first guess will help the operation to converge.
  - Select a reasonable step size & tolerance.
  - You can use the case study tool to determine the nature of the relationship between the dependant and independent variables.

Case Studies

- Varies Independent Variable(s) over a range (or in discrete states)
- Records the value of Dependant variables for each combination

Case Study Example

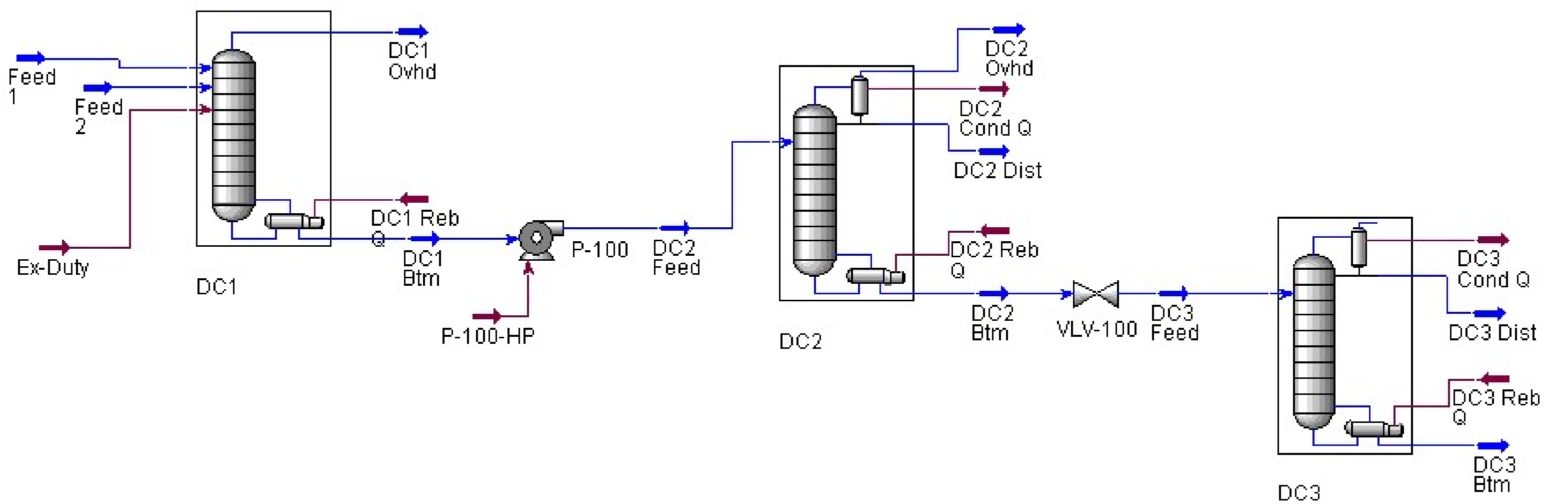
- 2 Stage Refrigeration Loop Example
  - Vary interstage pressure and record total compressor duty



Module 4 – NGL Fractionation Train

- Objectives:
  - Learn how to add columns (use input expert)
  - Understand column specifications and DOF.
- Some Tips on Columns
  - Every column has its own sub-flowsheet and its own solver.
  - Usually it is not necessary to enter the column sub-flowsheet, but you can create more complex setup by working in the column environment.
  - The column solver is a simultaneous solver; all items within the column flowsheet are solved together.
  - The pressure profile must be defined before the column can run. Also, all feed streams must be known.
  - You must hit the “Run” button to start the solver.

Module 4 – The Process



Module 5 – Oil Characterization

- Objectives:
  - Understand how to characterize an oil in UniSim Design
  - Learn how UniSim Design converts lab data into a series of hypothetical components for use in the simulation.

Oil Characterization Basics

- Step 1 – Enter the Assay Data
  - Assay data can be in one of many forms (TBP, D86, D2887, Chromatographic, etc.)
  - Light ends information can be included, estimated, or ignored.
  - Bulk property data can be entered, if available.
  - Other physical property curves (density, MW, viscosity) can be entered
- Step 2 – Blend and Cut the assays
  - You can blend several assays together (some times called ‘back-blending’).
  - You can specify one of three options for cutting the blends
    - Autocut – UniSim Design uses a default rule to cut the blend.
    - User points – The user enters the number of cuts that they want.
    - User ranges – The user enters the number of ranges and cuts per range.
- Step 3 – Install the Oil
  - Simply specify the stream that will carry the composition in the simulation environment.

Honeywell

Tips on Oil Characterization

- It is good to understand the correlations that UniSim Design will use to generate the hypocomponent properties.
- The Composite Plot can be used to test the accuracy of the curves (comparing user entered data with calculated data).
- The Distribution plot can be used to predict column product rates.
- The user should know how the lab data was obtained.
  - What type of analysis was done?
  - Were the light ends included?
- If bulk property data is available, it is good to use it.

Module 6 – Two Stage Compression

- Objectives:
  - Understand the use of the Recycle operation in UniSim Design.
  - Use the Simulation Balance Tool.
  - Understand proper usage and limitations of the pipe segment operation.

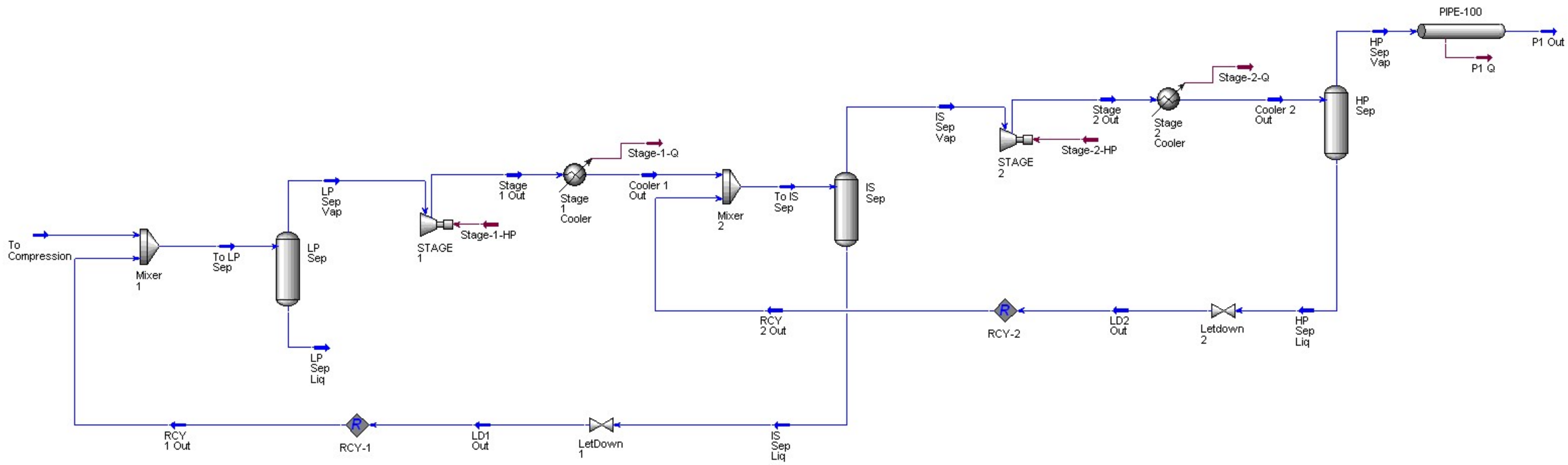
- Intro to the Recycle Operation
  - A mathematical operation that is required to allow the sequential modular simulator to solve.
  - Allows the user to 'guess' an outlet stream, then iterates until convergence is achieved.
  - Required any time a stream is returned back to an upstream point.

Module 6 – Two Stage Compression

- Intro to the Simulation Balance Tool
  - The Simulation Balance Tool (SBT) allows the user to perform overall mass and energy balance checks.
  - The SBT can reveal modeling errors even if the simulation appears to be fully converged.

- Intro to the Pipe Segment
  - Can solve for pressure drop, length, diameter, or flow.
  - Several options for two-phase flow correlations
    - Beggs and Brill – most commonly used.
    - Gregory Aziz Mandhane – also commonly used.
    - Neither B&B or GAM are applicable to every situation!
  - Heat transfer can be specified or estimated.

Module 6 – The Process



Recycle Positioning

- Do not necessarily represent a physical material recycle, often the physical recycle stream is not the best choice

- Recycles should be placed
  - So as to minimize the number of recycle operations
    - After mixing points (mixer)
    - Before separation points (tee, vessel, column)
  - Where as many parameters as possible are defined
  - In a stable stream

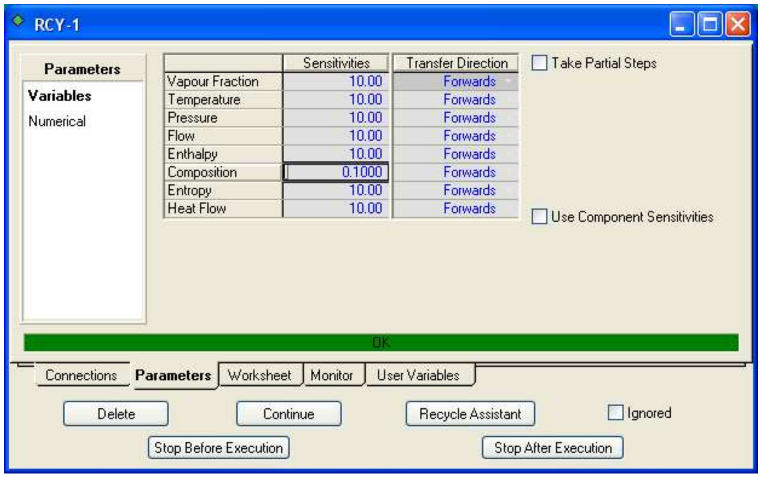
- When adding a Recycle - make a copy of the 'tear' stream first, and use this copy as your initial guess

Key Parameters

- The tolerances displayed in the Recycle operation are “sensitivities” that are multiplied by an internal tolerance to give the actual tolerance.

Property	Absolute tolerance	Internal Units
Vapour Fraction	0.01	
Temperature	0.01	°C
Pressure	0.01	kPa
Flow	0.001 (this is a relative error)	kgmole/s
Enthalpy	1	kJ/kgmole
Composition	0.0001	

Tolerance = Tolerance Sensitivity x Absolute Tolerance



Honeywell

Introduction to Simulation Balance Tool

- The Simulation Balance Tool (SBT) allows the user to perform overall mass and energy balance checks.

- The SBT can reveal modeling errors even if the simulation appears to be fully converged.

- Once run the SBT also provides an Overall Mass Balance Monitor, located on the status bar, giving a live indication of the status.

- Tolerance settings are used to specify which balances to perform and the checking tolerance used by the SBT in the validation.

Honeywell

Viewing Results in the SBT

- Results may be viewed in the following tabs:
  - Summary tab – General
    - Displays all unit operations where the specified balances exceed the specified tolerances.
    - Columns in between the absolute and relative error columns contain arrows to indicate which error(s) exceed the specified tolerance.
  - Summary tab – Detailed
    - Provides a unit-by-unit balance summary in terms of both absolute and relative errors. Double-clicking on the unit operation name(s) listed here will bring up the property view for that operation.
  - Feed/Products tab
    - Displays the overall mass and energy flows of all the feed and product streams in the simulation, and the overall balance errors. Green = within specified tolerances, Red = errors exceed the specified tolerances.

Viewing Results in the SBT (continued)

- Transitions tab
  - Shows all Transition objects (include recycle unit operations, flowsheet boundaries and stream cutters) with balance errors larger than the specified tolerances.
- Adjust/Recycle tab
  - Lists all Adjust and Recycle ops in the simulation with their key parameters.
- Select Normal to list objects by row, or Transpose to list by column.
- Alerts tab
  - Lists all unit operations in the simulation which have warning or error status messages.

Introduction to the Pipe Segment

- The Pipe Segment is used to simulate a wide variety of piping situations ranging from single or multi-phase piping with rigorous heat transfer estimation, to large capacity looped pipeline problems.
- The pipe segment offers four calculation modes:
  - Pressure Drop, Length, Flow, Diameter.
  - The appropriate mode will be automatically selected depending on the information supplied.
- Two-phase flow pressure drop correlations developed by Gregory, Aziz, and Mandhane, and Beggs and Brill (default), among others, are offered.
- For single phase streams, the Darcy equation is used for pressure drop predictions, regardless of the correlation selected on the Parameters page.
- Heat transfer data can be specified or estimated.
- On the Sizing page of the Rating tab, the user constructs the length-elevation profile for the pipe segment. To fully define the pipe section segments, the pipe schedule, diameter, material and # of increments must also be specified.

Honeywell

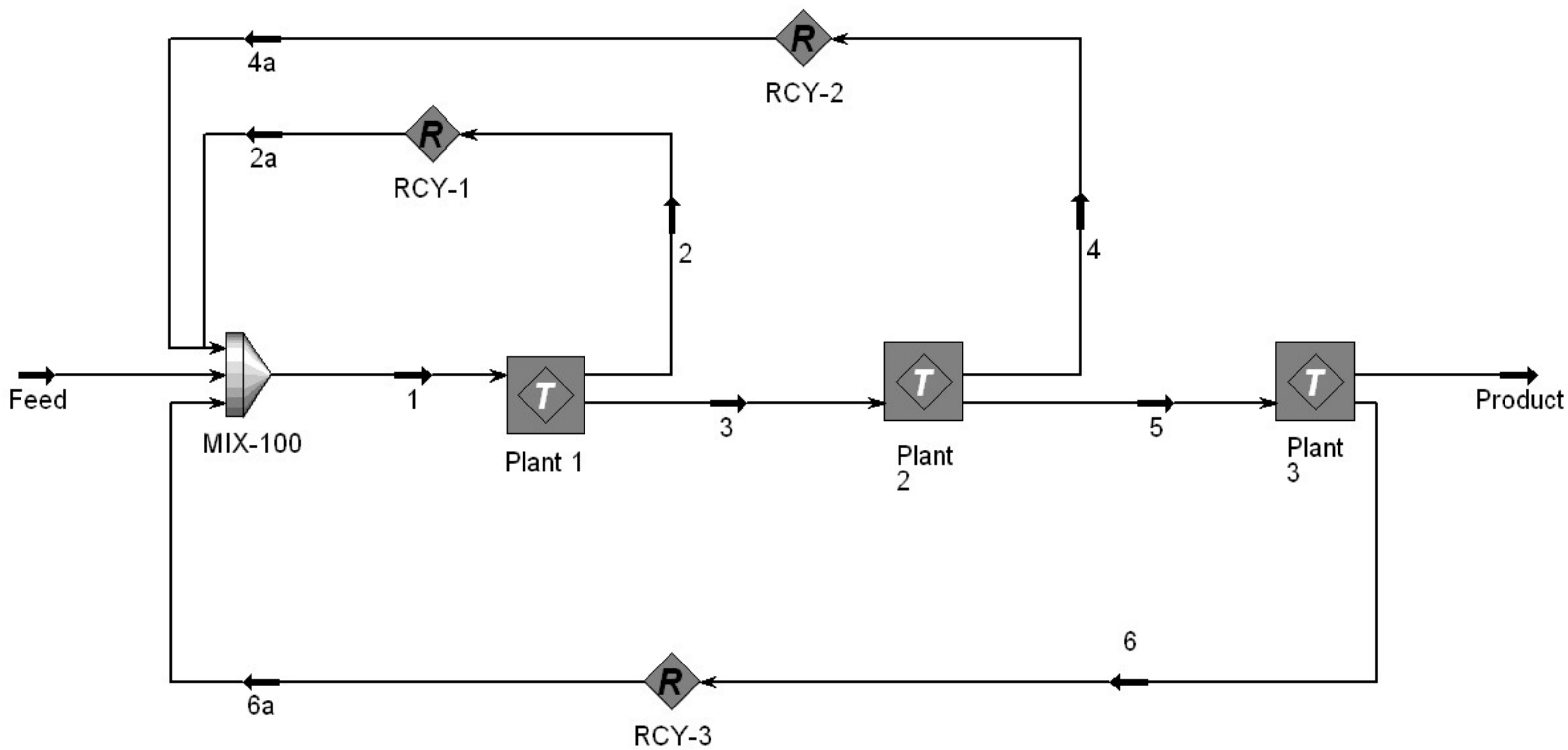
Module 6 – The Exercises

- Three Questions for each Exercise

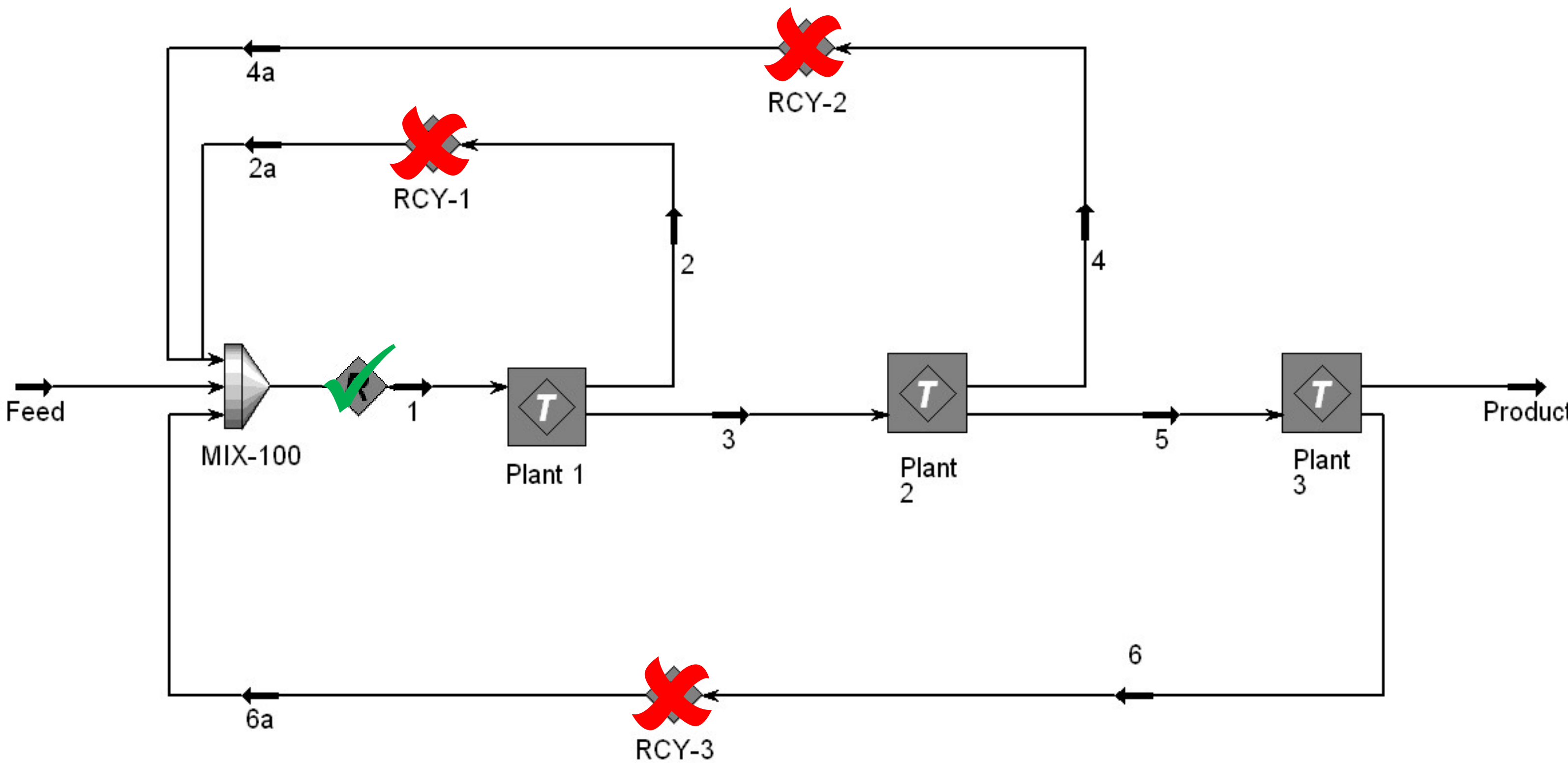
1. Does this process require a recycle operation?
2. If yes, then how many?
3. Where should they be located?

- Note:
  - Number of Recycles required does not only depend on the flowsheet configuration
  - Type / Positioning of Specifications is also important

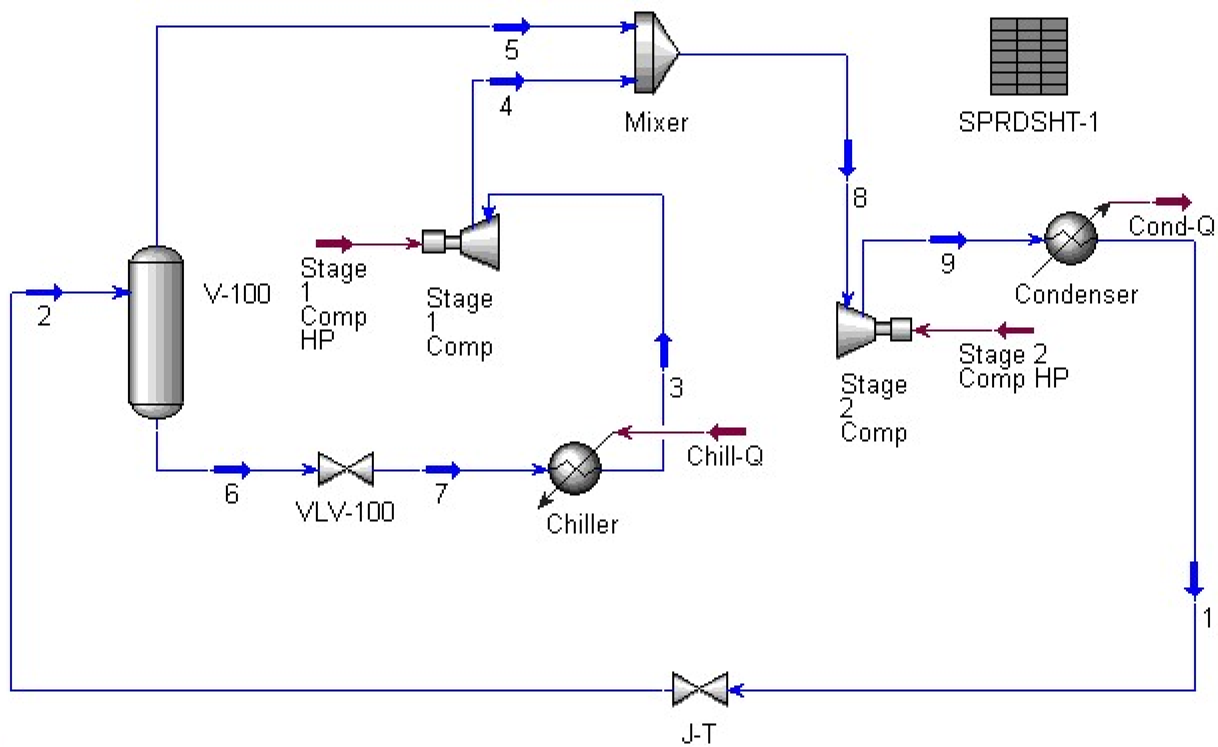
Module 6 – Exercise 1



Module 6 – Exercise 1 – Answer

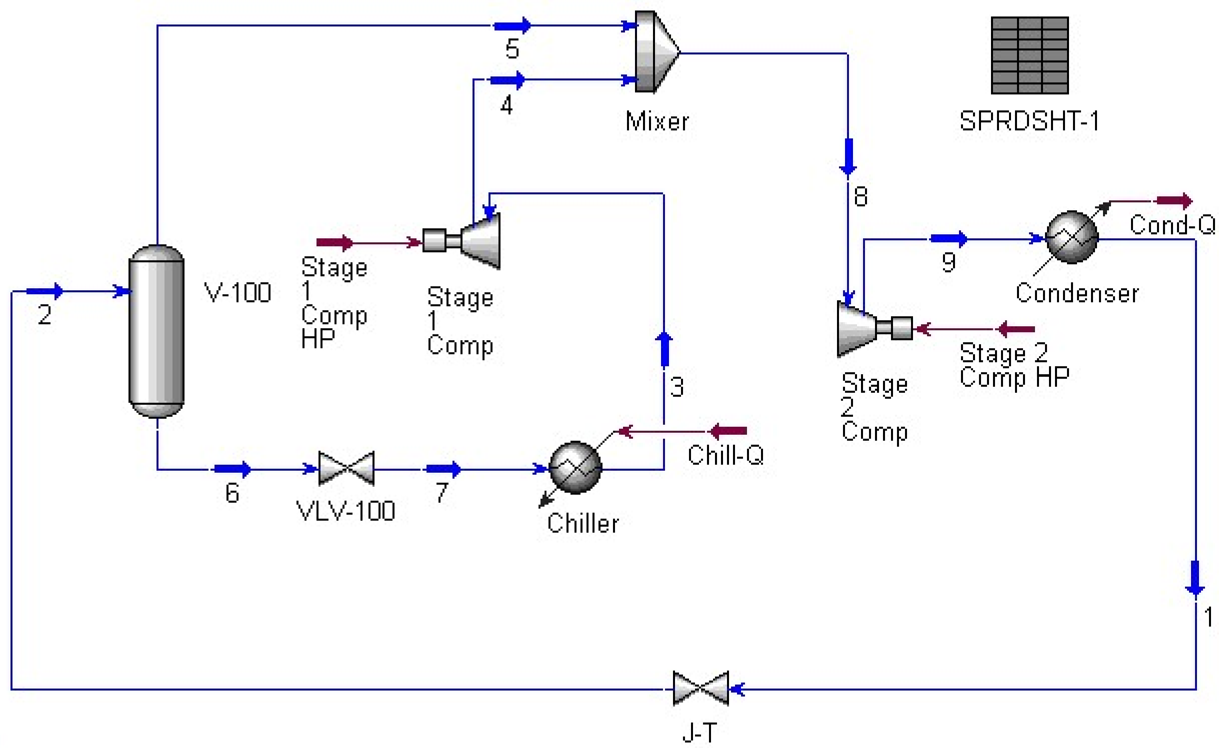


Module 6 – Exercise 2

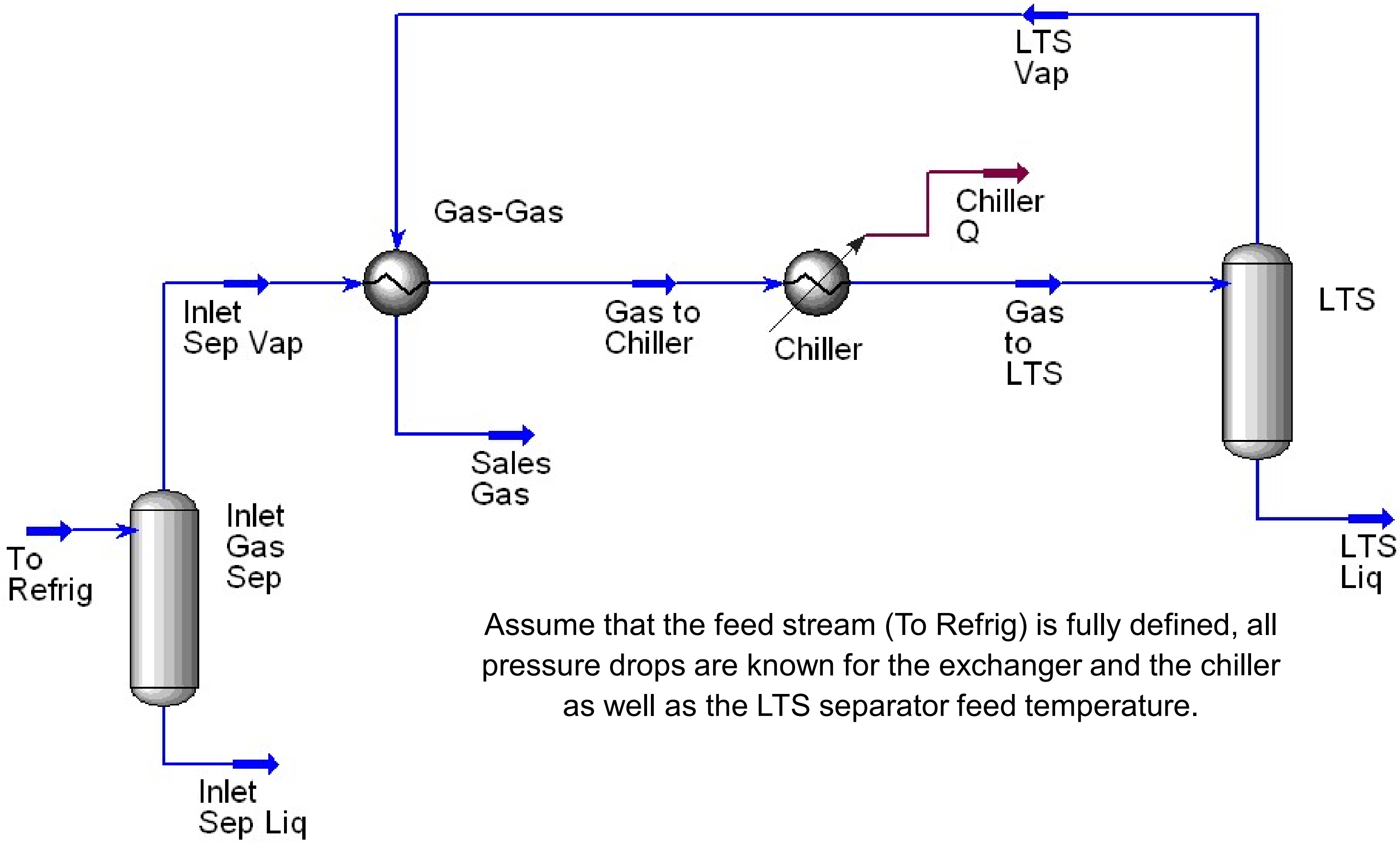


Module 6 – Exercise 2 – Answer

- No Recycle needed



Module 6 – Exercise 3

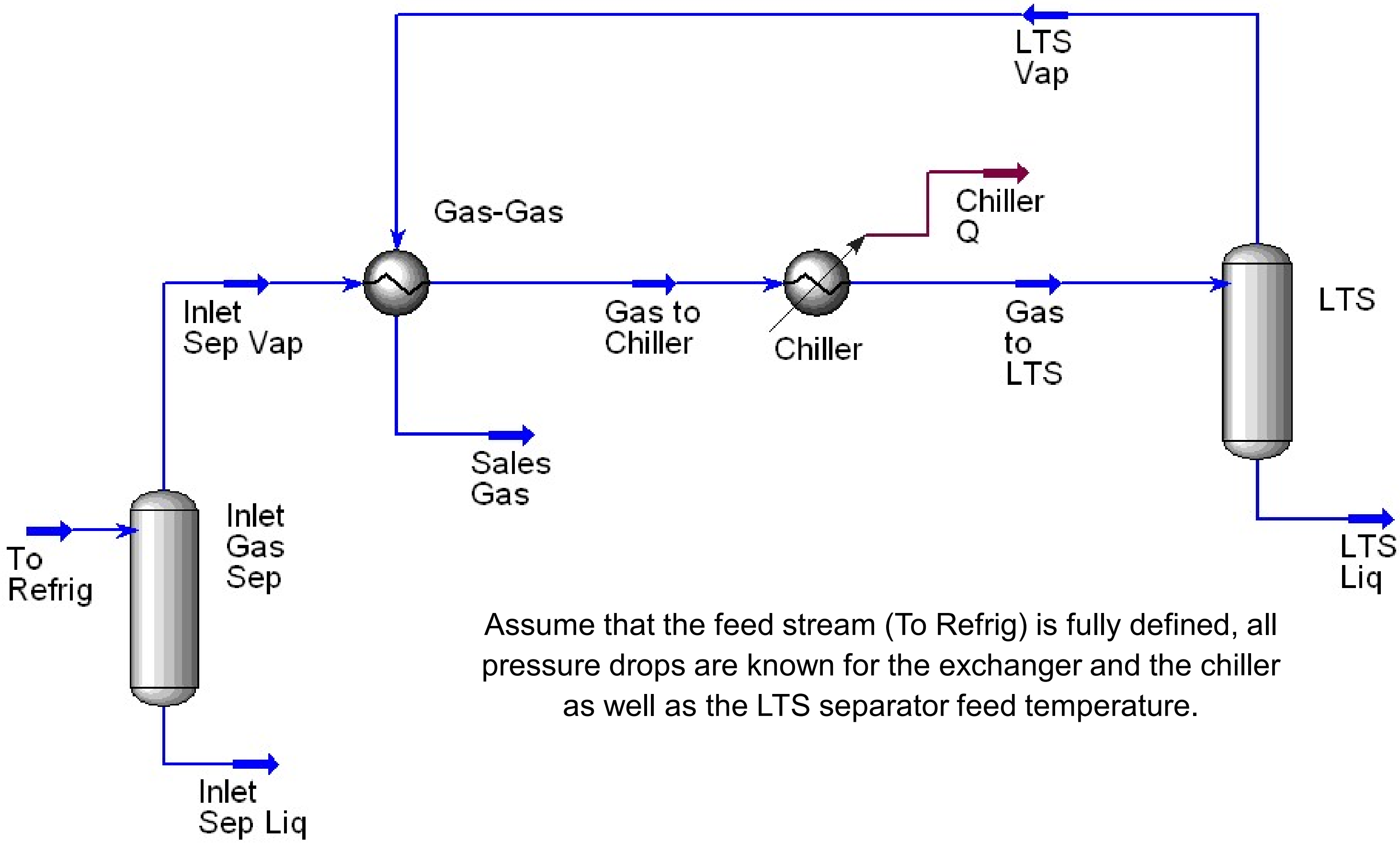


Assume that the feed stream (To Refrig) is fully defined, all pressure drops are known for the exchanger and the chiller as well as the LTS separator feed temperature.

Honeywell

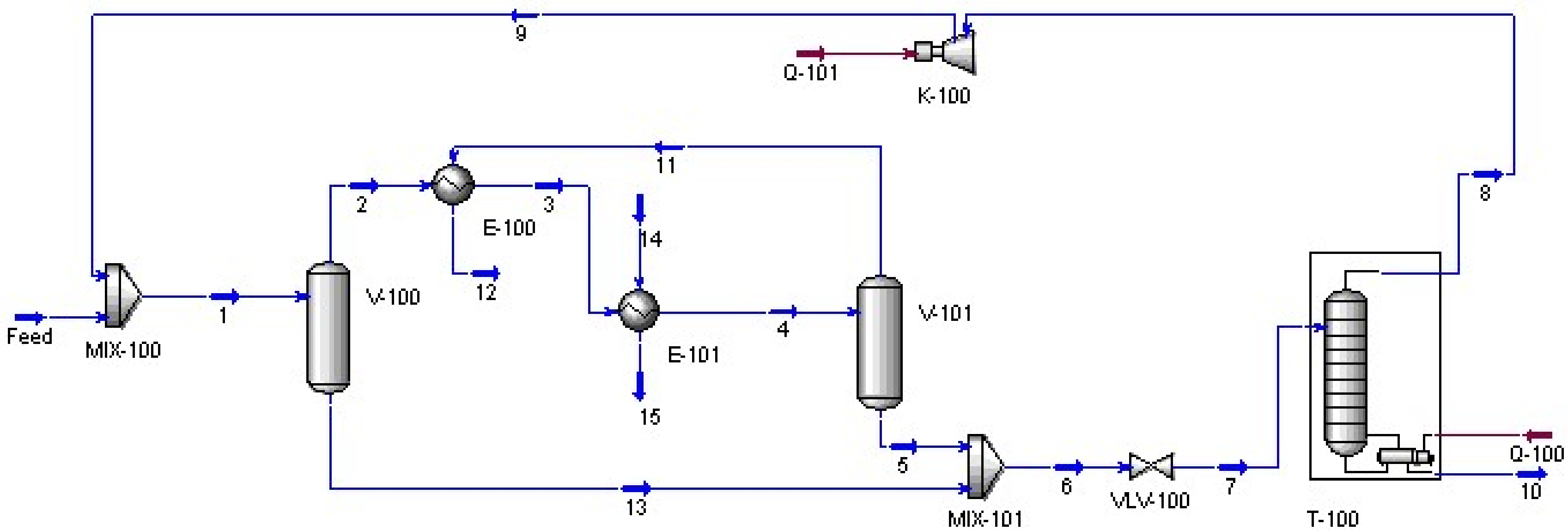
Module 6 – Exercise 3 – Answer

- No Recycle Needed



Assume that the feed stream (To Refrig) is fully defined, all pressure drops are known for the exchanger and the chiller as well as the LTS separator feed temperature.

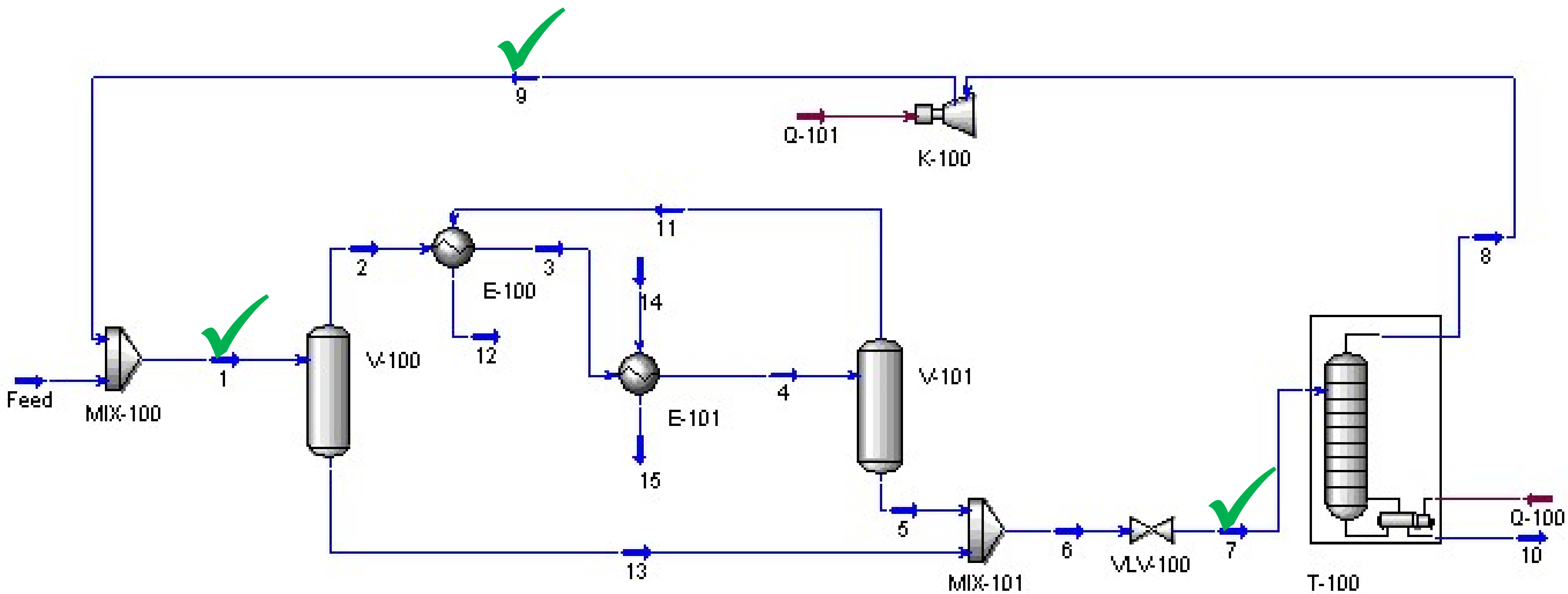
Module 6 – Exercise 4



Assume the Feed is completely defined. Also known are the shell and tube side pressure drops for E-100 and E-101, and the temperatures of streams 3 and 4.

Module 6 – Exercise 4 – Answer

- <u>One</u> Recycle in any of these locations



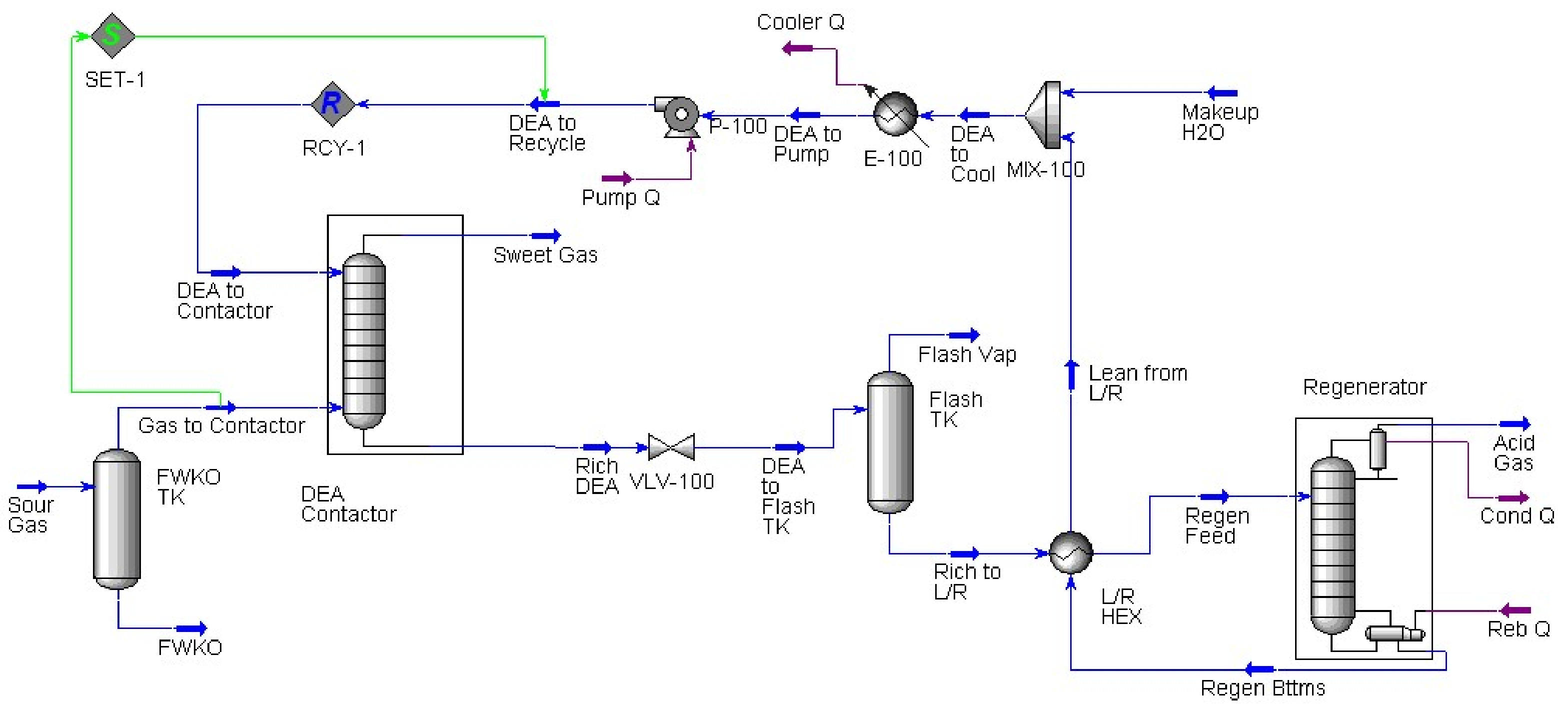
Assume the Feed is completely defined. Also known are the shell and tube side pressure drops for E-100 and E-101, and the temperatures of streams 3 and 4.

Honeywell

Module 7 – Acid Gas Sweetening with DEA

- Objectives:
  - Understand the proper usage and limitations of the Amine Package in UniSim Design.
  - Use the Spreadsheet operation to calculate the lean and rich amine loading factors.

Module 7 – The Process



Introduction to the DBR Amine Package

- Uses the Amine Thermodynamic Model in UniSim Design.
- Based on AMSIM, a product from Schlumberger.
- Uses a non-equilibrium stage model to simulate mass transfer processes in Amine contactor and regenerators.
- Calculates component based efficiencies based on liquid and vapour rates and tray geometry.
- Amine solubility and kinetic data based on a mixture of published and unpublished data.

DBR Amine Package Limitations

- Limited Component Database
  - Amines: MEA, DEA, TEA, MDEA, DGA, DIPA
  - Acid Gases: CO_2, H_2S, COS, CS_2
  - Paraffins: C1 to C12
  - Olefins: C2=, C3=, C4=, C5=
  - Mercaptans: M-Mercaptan, E-Mercaptan
  - Inerts: H_2, N_2, O_2, CO, H_2O
  - Hypothetical components are NOT allowed.
  - Valid only with certain ranges:
    - MEA: 0-30 wt% Amine
    - DEA, MDEA & TEA: 0-50 wt% Amine
    - DGA: 50-70 wt% Amine
    - DIPA: 0-40 wt% Amine
    - Temperature: 25°C – 125°C
    - Pressure = 0 kPa – 2100 kPa

Tips for Using the Spreadsheet

- Use the Spreadsheet tab directly. Do not use the Connections tab or the Formulas tab.
- Cells can contain four types of data:
  - Text (Comments)
  - Specified values
  - Imported variables
  - Calculated variables
    - (Only Calculated variables are "exportable")
- You can add additional rows and columns on the Parameters tab.
- The Spreadsheet can use a different unit set, but will 'lock' whatever unit set it is using.
- Use variable names to help identify key cells.

Honeywell

Examples of Spreadsheet Uses

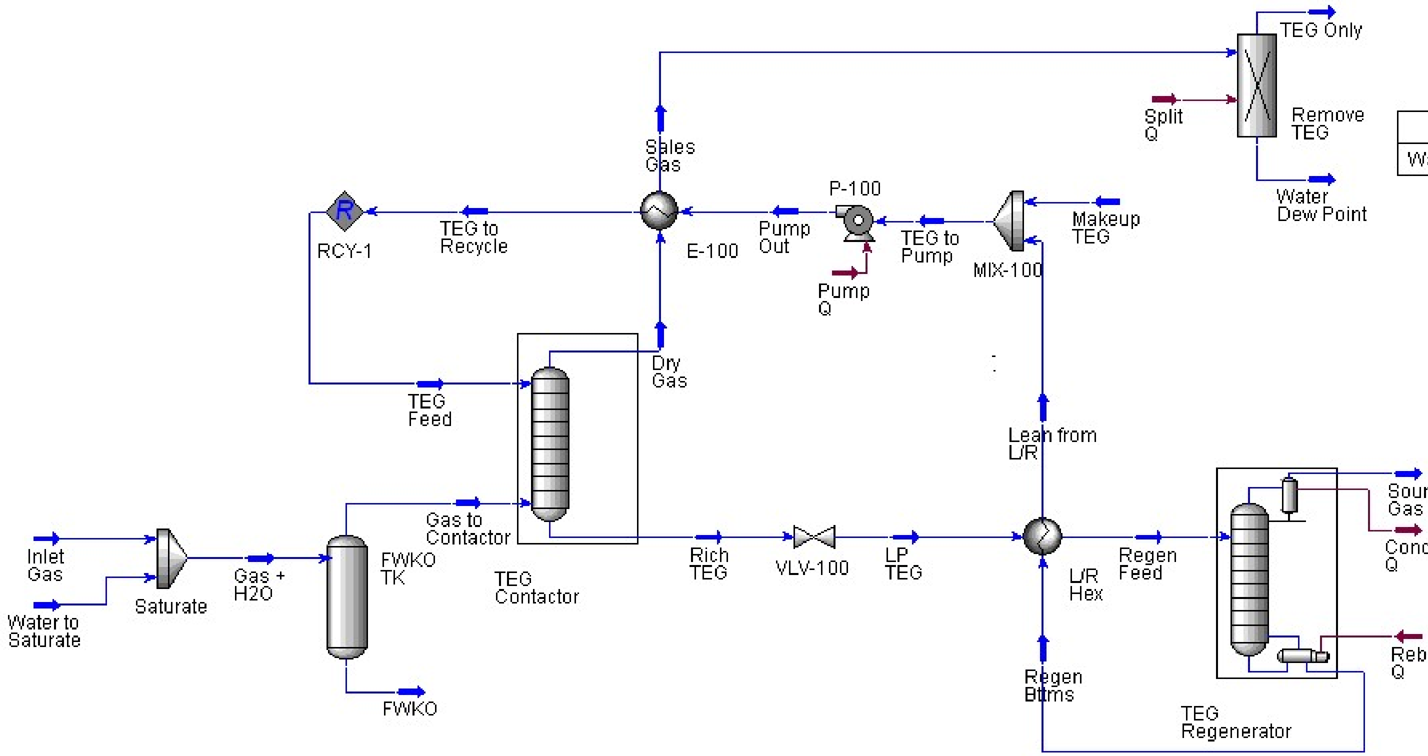
- Summary of key input / output values
- Create simple “input forms”
- Gather similar data from several sources (e.g. a plant pressure profile)
- To do non standard calculations – e.g. Cost and Profit calculations
- Do calculations on imported variables and export the results back to the process. For example, import the flow through a heat exchanger, calculate a deltaP and export the result back to the heat exchanger.

Honeywell

Module 8 – Natural Gas Dehydration with TEG

- Objectives:
  - Model a typical TEG Dehydration Unit in UniSim Design.
  - Calculate the Water Dew point for a stream in UniSim Design using the Water Dew Point Property Correlation.

Module 8 – The Process



Water Dew Point		
Water Dew Point	-13.89	C

Honeywell

Module 9 – Reporting in UniSim Design

- Objectives:
  - Look at several methods of retrieving data out of UniSim Design.

- The Methods Are:
  - Customizing the Workbook
  - Printing the datasheet
  - Adding process data to the PFD
  - Using the Copy-Paste functionality to get the data into Excel
  - Using Excel based Macros