Process Simulation with ASPEN PLUS

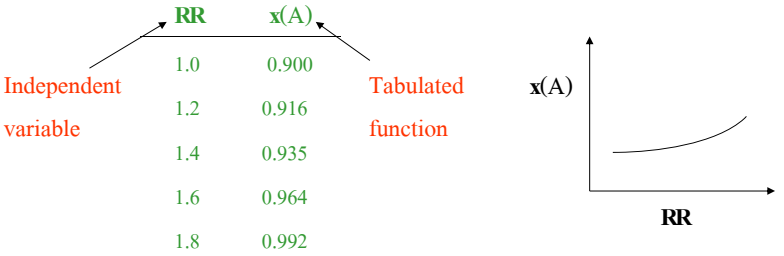
CHE654 Course Notes

Section 5: Sensitivity Analysis

These course materials are applicable to Version 8.4 of ASPEN PLUS

Sensitivity Analysis Feature

- Sensitivity analysis examines the variation of process results with changes to key flowsheet variables.
- Sensitivity generates tables in the base case report.



Setting up a Sensitivity Analysis Block

1. Identify the flowsheet variables to be sampled.
2. Select or compute the variables that are to be tabulated (dependent variable or tabulated function).
3. Identify the variables to be varied.
4. Select values for the independent variables.

Caution: Each combination of independent variable values requires one evaluation of the sensitivity block. For sensitivity blocks with several independent variables, the number of combination can be surprisingly large.

Setting up a Sensitivity Analysis (Cont'd)

$$\text{Total No. of Evaluations} = \prod_{i=1}^{N} \alpha_i$$

where **N** = total number of independent variables

α_i = total number of points in independent variable **i**

Example: 2 independent variables to vary T and P

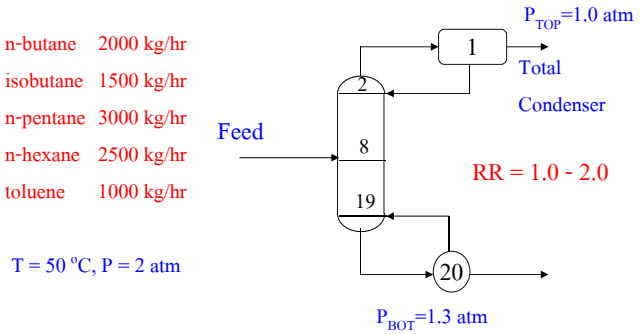
T(^{o}F) = 100, 200, 300, 400, 500

P(atm) = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10

No. of Combinations = (5)(10) = 50 points

Example of Sensitivity Analysis: DISTL Problem

- Recall the C_4 - C_7 separation problem using DISTL
- Use Sensitivity to study the effect of Reflux Ratio (RR) in DISTL on product purity, namely $\mathbf{x}_{butane}$ and $\mathbf{x}_{toluene}$



Sensitivity Example (Cont'd)

- Sensitivity feature is invoked by selecting Model Analysis Tools in Data pulldown menu.
- Fill out 1. Define tab => access variables from flowsheet
  2. Vary tab => identify manipulated variable
  3. Tabulate tab => select/compute variables to be tabulated

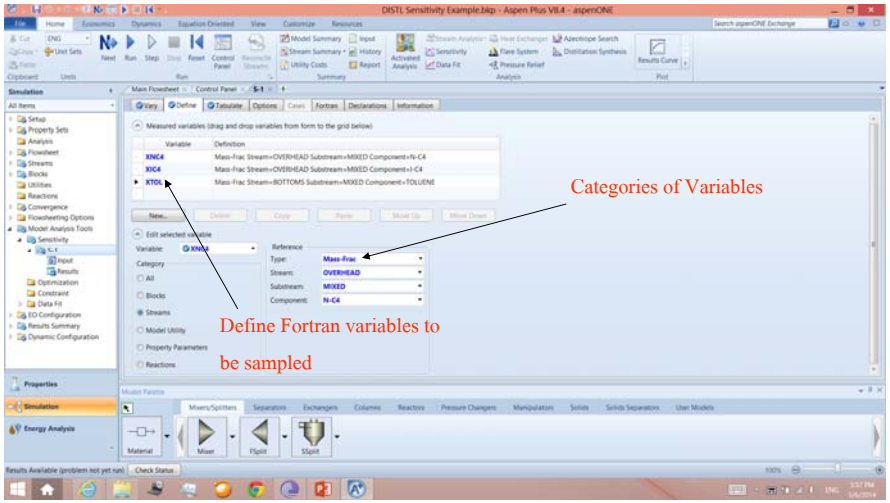
Accessing Variables

- Capability in A+ to sample or manipulate any desired block or stream variables
- Used primarily in Sensitivity, Case Studies, and Design-Spec
- Sampled variables
  - Any simulation block input/results, e.g. outlet temperature, block pressure
  - Any stream variable, e.g. mole fraction of a component
- Manipulated variables
  - Any block input such as distillation reflux ratio
  - Any stream input such as component feed flow

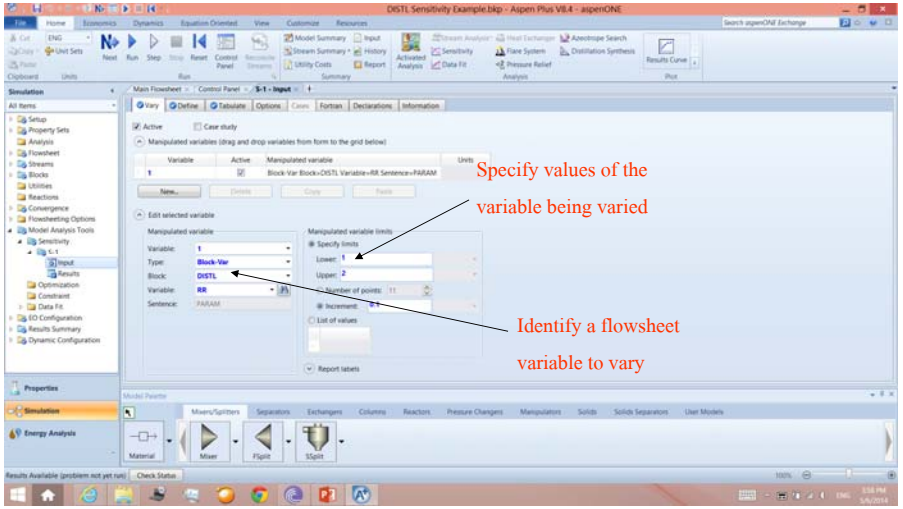
Important Categories of Variables

- Blocks Category
  - Block-Var Type: Access variables associated with block input/output, such as column RR, flash outlet T, reactor duty, etc.
- Streams Category
  - Stream-Var Type: Access standard properties of streams, such as T, P, total flow, enthalpy, molar volume, etc.
  - Mole-Flow or Mass-Flow Type: Access component flow rates of streams
  - Mole-Frac or Mass-Frac Type: Access mole/mass fractions of components in a stream
  - Stream-Prop Type: Access non-standard properties (PROP-SET) of a stream, such as viscosity, surface tension, heat capacity, etc.
- Property Category
  - Access physical property parameters

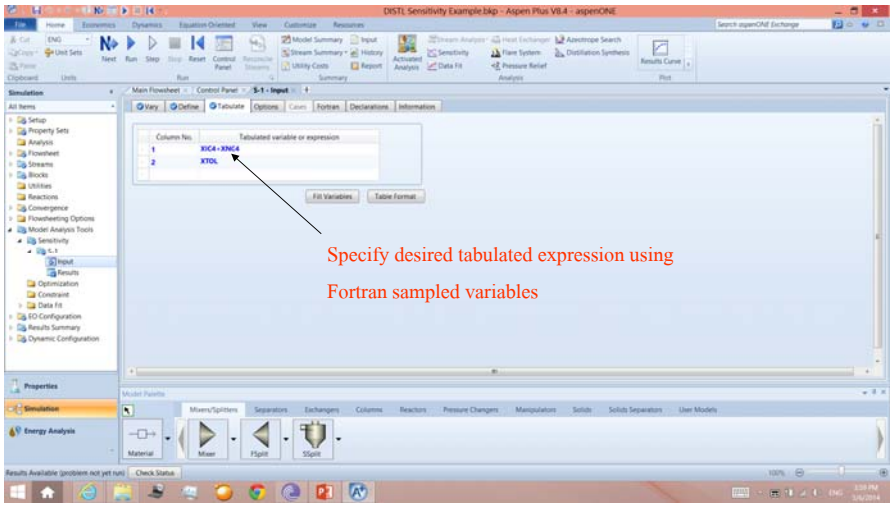
Define Tab in Sensitivity



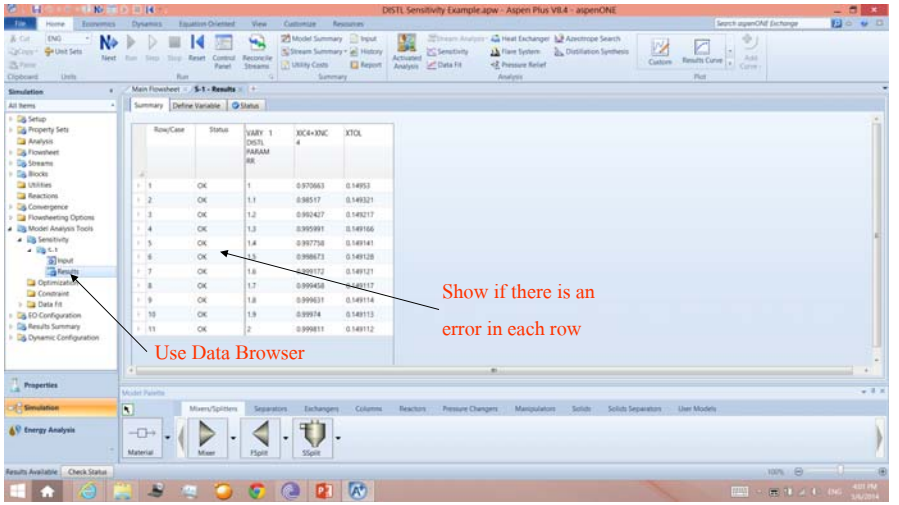
Vary Tab in Sensitivity



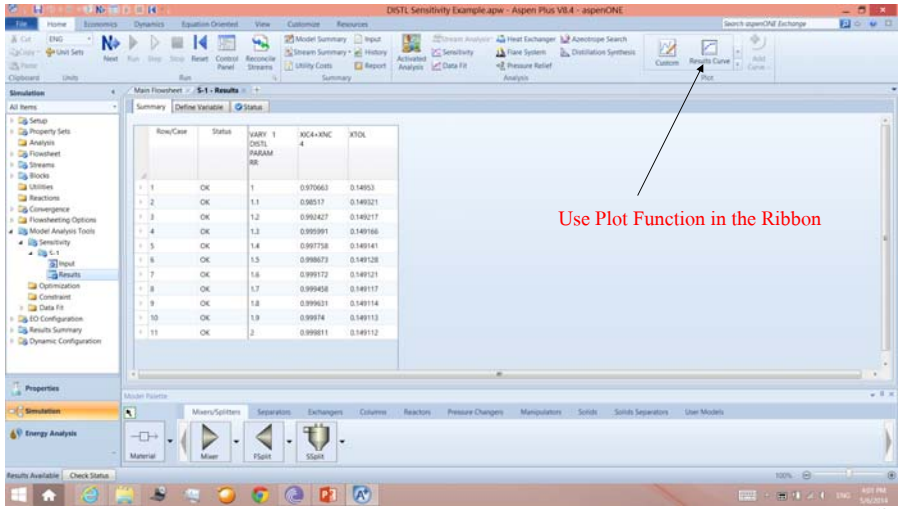
Tabulate Tab in Sensitivity



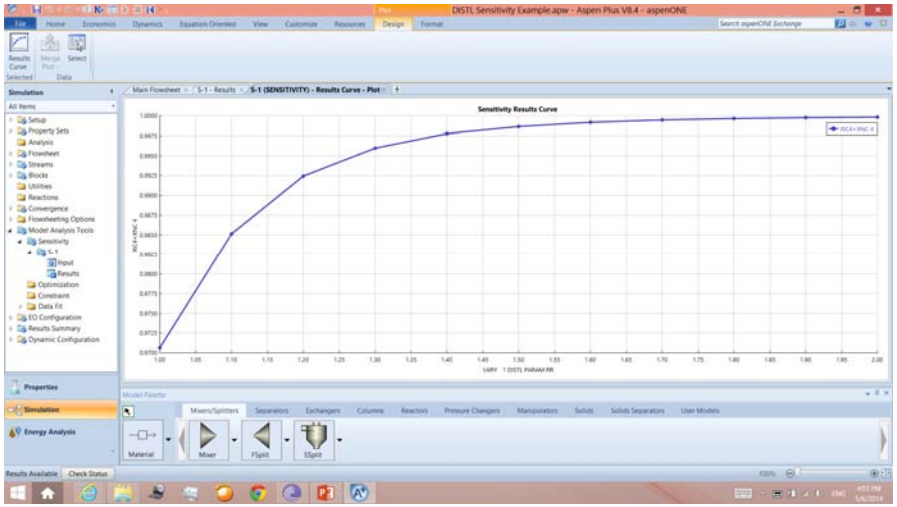
Viewing Sensitivity Results



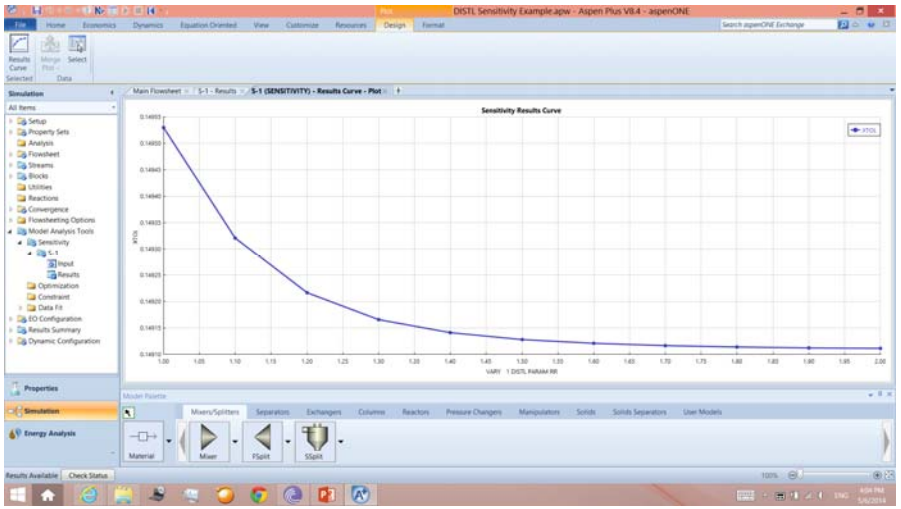
Plotting Sensitivity Results



Sensitivity Plot #1

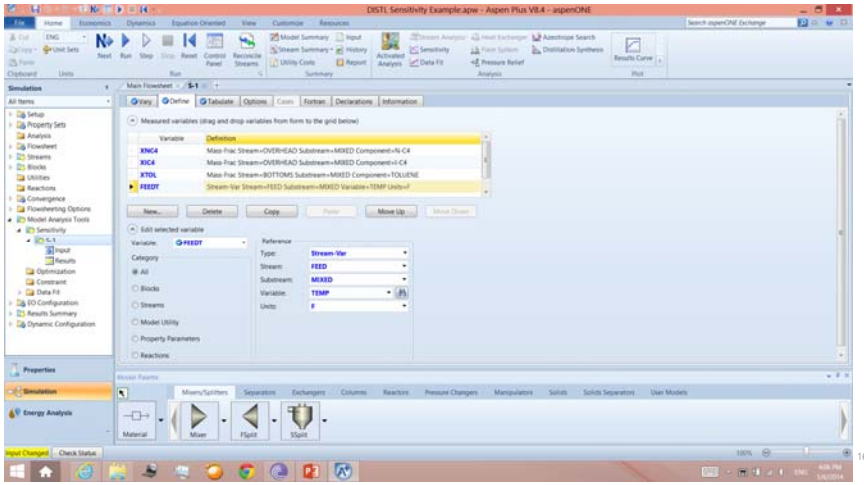


Sensitivity Plot #2



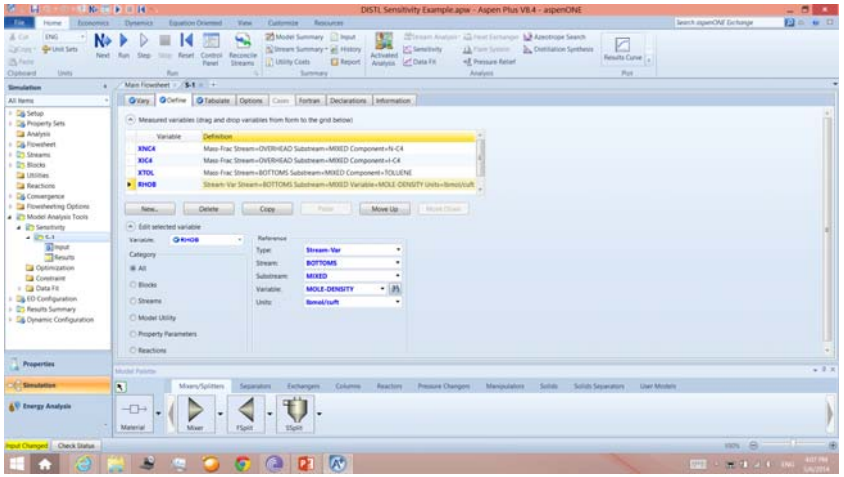
Examples of Accessing Variables

Example 1: Access the temperature of a stream called FEED



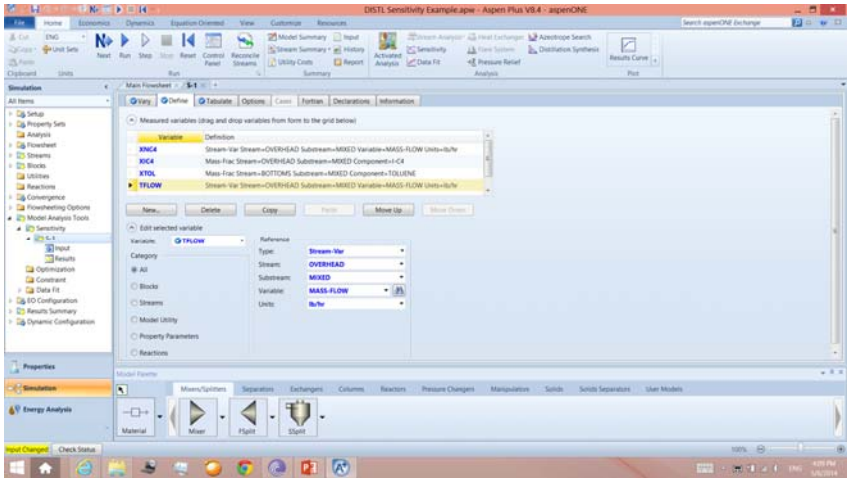
Examples of Accessing Variables (Cont'd)

Example 2: Access the molar density of a stream called BOTTOMS



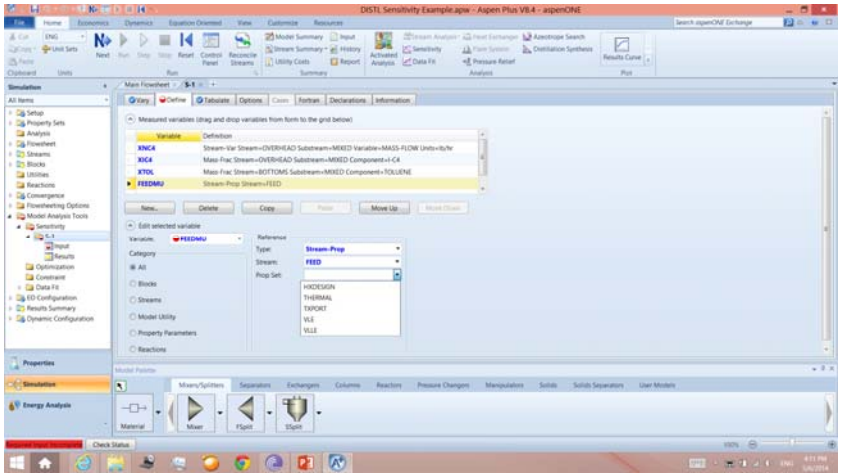
Examples of Accessing Variables (Cont'd)

Example 3: Access the total mass flow of a stream called OVHDS



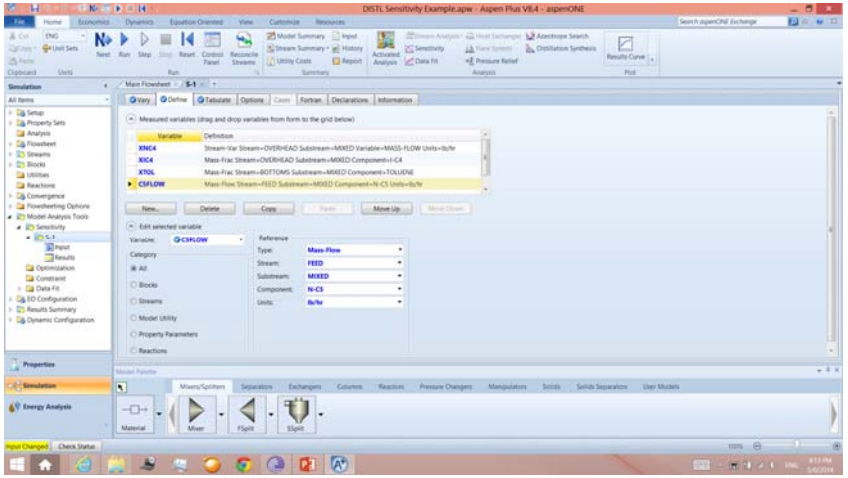
Examples of Accessing Variables (Cont'd)

Example 4: Access the viscosity of a stream called FEED



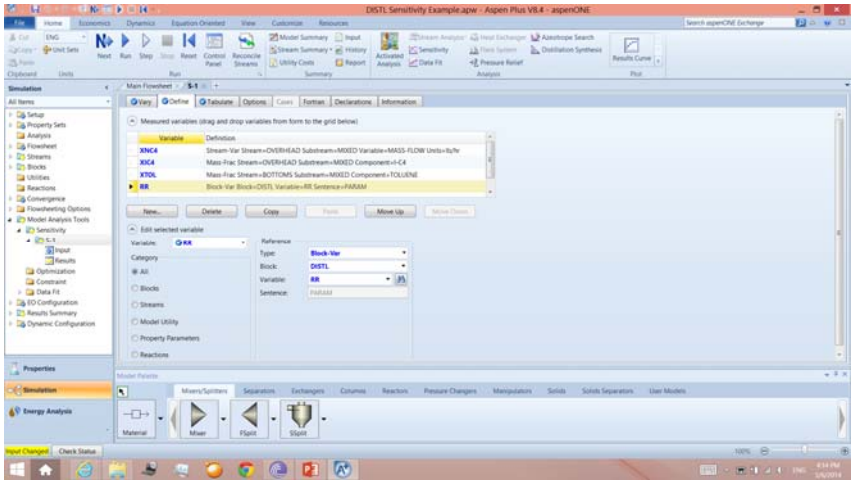
Examples of Accessing Variables (Cont'd)

Example 5: Access the mass flow of component C5 in stream FEED



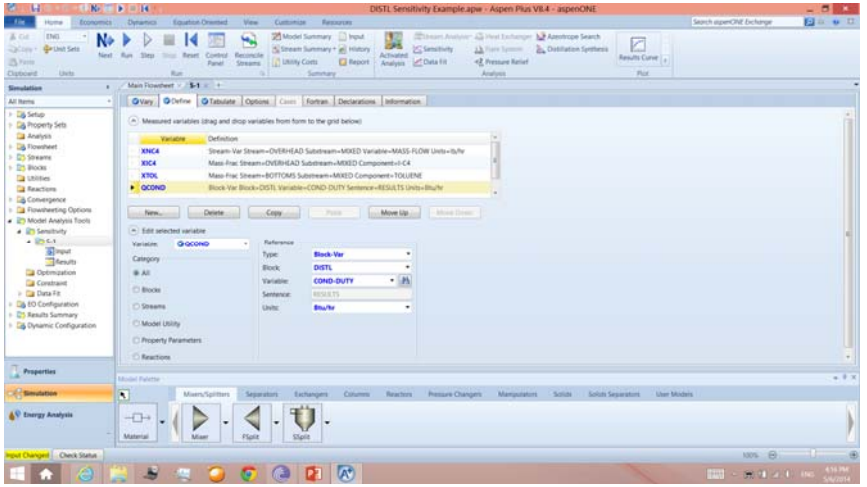
Examples of Accessing Variables (Cont'd)

Example 6: Access the reflux ratio (input) of a DISTL block



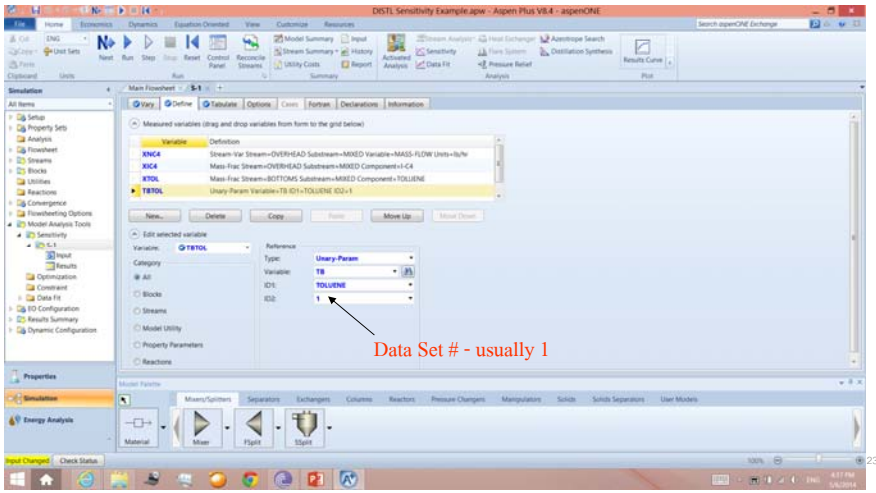
Examples of Accessing Variables (Cont'd)

Example 7: Access the condenser duty (result) in a DISTL block



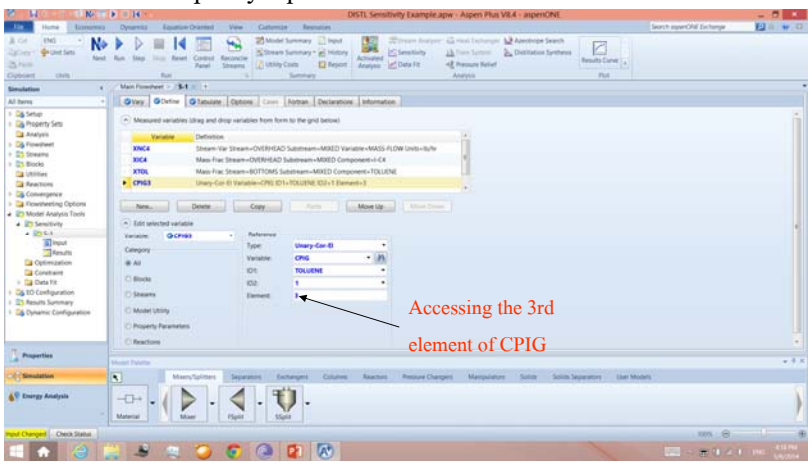
Examples of Accessing Variables (Cont'd)

Example 8: Access the normal boiling point of component TOLUENE



Examples of Accessing Variables (Cont'd)

Example 9: Access the 3rd element or coefficient in the ideal gas heat capacity equation of TOLUENE



Ideal Gas Heat Capacity Equation in A+

- A+ contains many physical property parameters which are in the form of equations or correlations.

- For example, CPIG is the ideal gas heat capacity with 11 elements (coefficients)

$$C_P^{IG} = C_1 + C_2 T + C_3 T^2 + C_4 T^3 + C_5 T^4 + C_6 T^5 \quad \text{for } C_7 \leq T \leq C_8$$

$$C_P^{IG} = C_9 + C_{10} T^{C11} \quad \text{for } T < C_7$$

Sampled Variable vs. Manipulated Variable

- All flowsheet variables (both input and results) can be sampled.
- But only certain flowsheet variables can be manipulated.
- Examples: Can we manipulate the following?
  - The total flow of stream OVHDS?
  - The mass fraction of C6 in stream BOTTOMS?
  - The flow rate of TOLUENE in stream FEED?
  - The molar volume of stream FEED?
  - The reflux ratio of the DISTL column?
  - The condenser duty of the DISTL column?
  - The feed tray location?
- Allowed to adjust or manipulate flowsheet input only !!!

Fortran and Declaration Tabs

- The Fortran tab is used to enter Fortran executable statements for use in the Sensitivity Analysis.

- The Declaration tab is used to enter Fortran declaration statements such as declaring real and integer variables, and dimensioning arrays and vectors.
  - Examples:
  - REAL*8 TRAYT(30) => Declaring a real variable TRAYT as a vector with 30 elements
  - INTEGER NS(5) => Declaring an integer variable NS as a vector with 5 elements
  - REAL*8 SAT(5,10) => Declaring a real variable
  - REAL*8 KVL => Forcing a variable KVL to be a real number

Some Fortran Tips

1. All variables are limited to 6 characters or less.
2. A variables can consist of alphabets and numbers, but may not start with a number. In A+, do not begin variable names with IZ or ZZ.
3. By default, variables starting with a character between A-H and O-Z are real numbers (e.g. 1.42532), while those starting with a character between I-N are integer numbers.
4. All Fortran executable statements must start on column 7 or after.
5. Column 1 is reserved to indicate a comment line (and leave column 2 blank).
6. Column 6 is reserved to indicate a continuation line.

Workshop 3A: VCM Sensitivity Analysis

- Go to Course Notes Section 9 and work on Workshop 3A.