

Process Simulation with ASPEN PLUS

CHE654 Course Notes

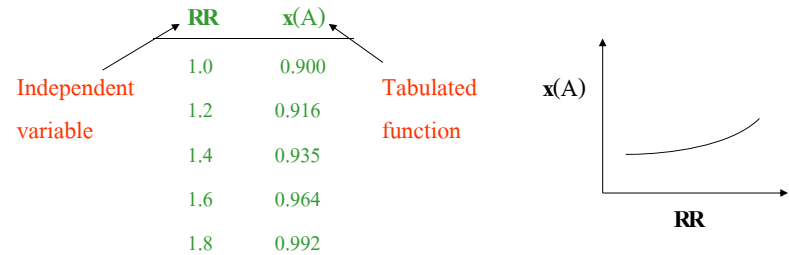
Section 5: Sensitivity Analysis

These course materials are applicable to Version 8.4 of ASPEN PLUS
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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.



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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.

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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(° F) = 100, 200, 300, 400, 500

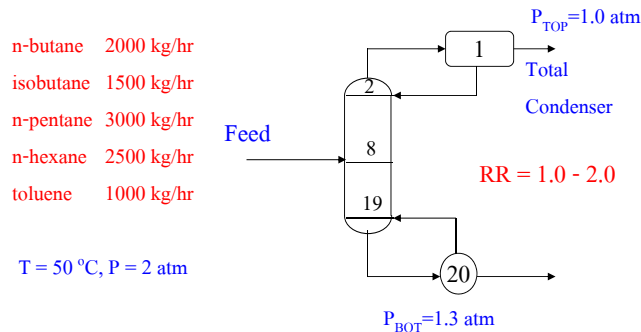
P(atm) = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10

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

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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 x_{butane} and x_{toluene}



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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
 - Vary** tab => identify manipulated variable
 - Tabulate** tab => select/compute variables to be tabulated

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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

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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

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Define Tab in Sensitivity

Categories of Variables

Define Fortran variables to be sampled

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Vary Tab in Sensitivity

Specify values of the variable being varied

Identify a flowsheet variable to vary

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Tabulate Tab in Sensitivity

Specify desired tabulated expression using Fortran sampled variables

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Viewing Sensitivity Results

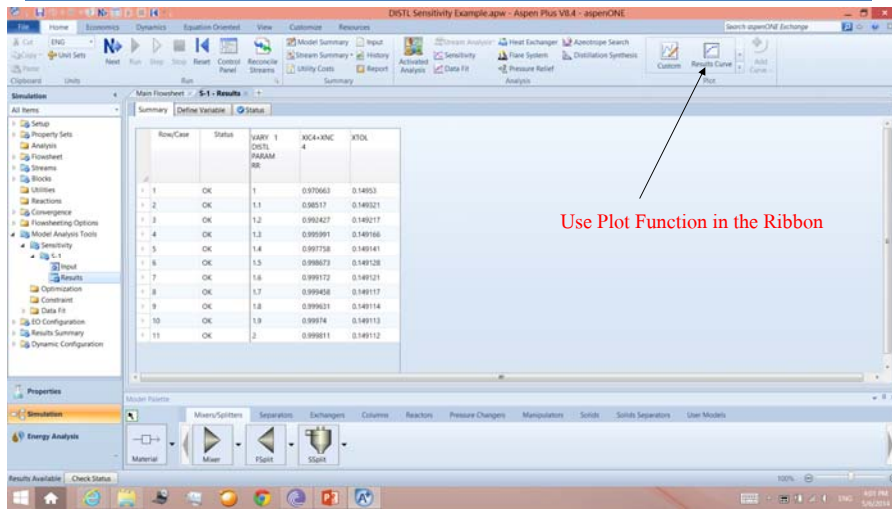
Row/Case	Status	VARY 1	KIC4-KNC4	XTOL
1	OK	1.0	0.975063	0.149133
2	OK	1.1	0.985117	0.149231
3	OK	1.2	0.992427	0.149217
4	OK	1.3	0.995981	0.149166
5	OK	1.4	0.997738	0.149141
6	OK	1.5	0.998673	0.149128
7	OK	1.6	0.999172	0.149121
8	OK	1.7	0.999458	0.149117
9	OK	1.8	0.999631	0.149114
10	OK	1.9	0.99974	0.149113
11	OK	2.0	0.999811	0.149112

Use Data Browser

Show if there is an error in each row

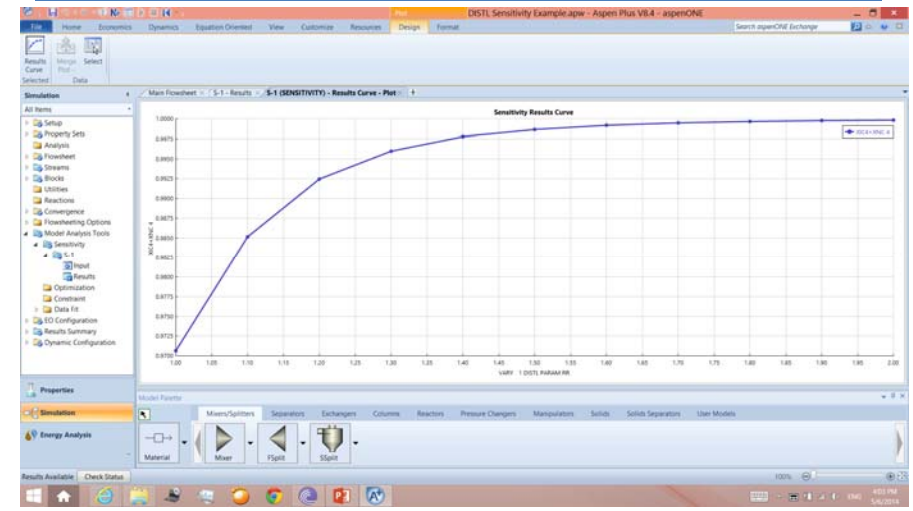
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Plotting Sensitivity Results



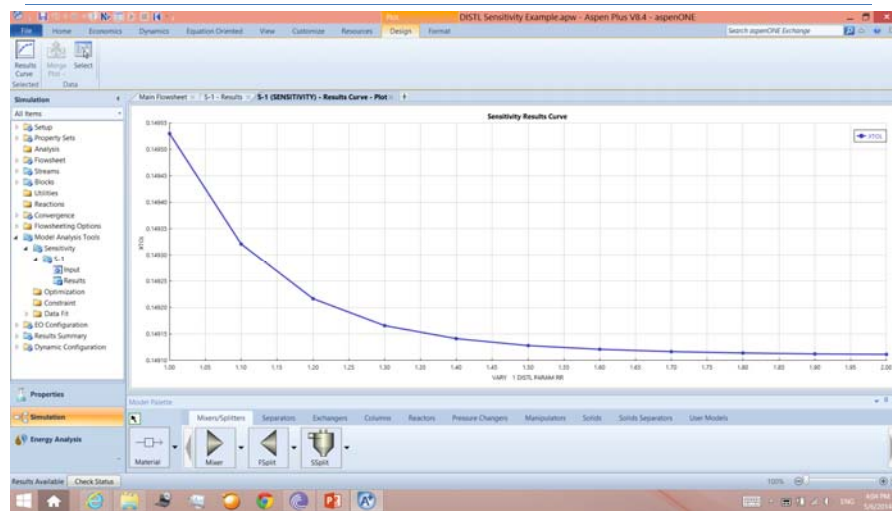
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Sensitivity Plot #1



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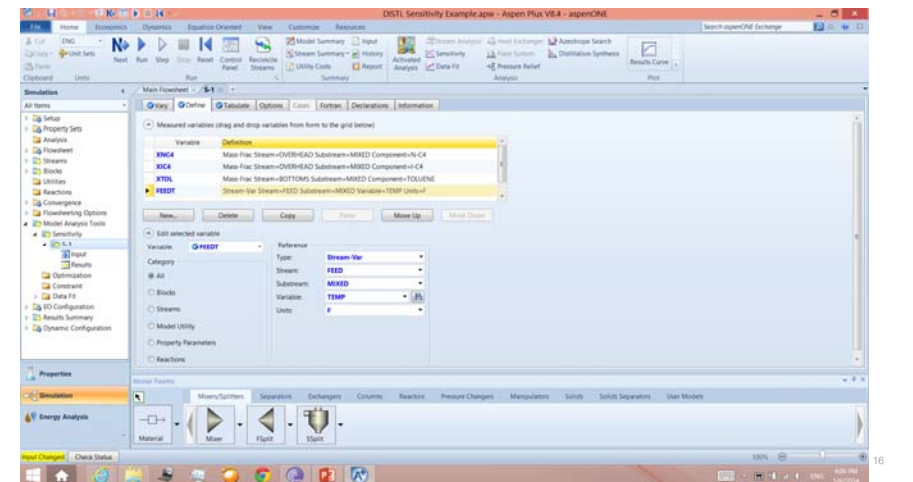
Sensitivity Plot #2



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Examples of Accessing Variables

Example 1: Access the temperature of a stream called FEED



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Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface with the 'Main FlowSheet' window. The 'Variables' list includes:

Variable	Definition
INCA	Mass Frac Stream=OVERHEAD Substream=MIXED Component=N-C4
NICA	Mass Frac Stream=OVERHEAD Substream=MIXED Component=I-C4
XTOL	Mass Frac Stream=BOTTOMS Substream=MIXED Component=TOLUENE
INCB	Stream Var Stream=BOTTOMS Substream=MIXED Variable=MOLE DENSITY Units=lbmol/ft ³

The 'Edit selected variable' window is open for 'INCB'. The 'Reference' is 'Stream Var', 'Type' is 'Stream Var', 'Stream' is 'BOTTOMS', 'Substream' is 'MIXED', 'Variable' is 'MOLE DENSITY', and 'Units' is 'lbmol/ft³'.

Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface with the 'Main FlowSheet' window. The 'Variables' list includes:

Variable	Definition
INCA	Stream Var Stream=OVERHEAD Substream=MIXED Variable=MASS-FLOW Units=lb/hr
NICA	Mass Frac Stream=OVERHEAD Substream=MIXED Component=I-C4
XTOL	Mass Frac Stream=BOTTOMS Substream=MIXED Component=TOLUENE
TFLOW	Stream Var Stream=OVERHEAD Substream=MIXED Variable=MASS-FLOW Units=lb/hr

The 'Edit selected variable' window is open for 'TFLOW'. The 'Reference' is 'Stream Var', 'Type' is 'Stream Var', 'Stream' is 'OVERHEAD', 'Substream' is 'MIXED', 'Variable' is 'MASS-FLOW', and 'Units' is 'lb/hr'.

Examples of Accessing Variables (Cont'd)

Example 4: Access the viscosity of a stream called FEED

The screenshot shows the Aspen Plus V8.4 interface with the 'Main FlowSheet' window. The 'Variables' list includes:

Variable	Definition
INCA	Stream Var Stream=OVERHEAD Substream=MIXED Variable=MASS-FLOW Units=lb/hr
NICA	Mass Frac Stream=OVERHEAD Substream=MIXED Component=I-C4
XTOL	Mass Frac Stream=BOTTOMS Substream=MIXED Component=TOLUENE
FEEDMU	Stream Prop Stream=FEED

The 'Edit selected variable' window is open for 'FEEDMU'. The 'Reference' is 'Stream Prop', 'Type' is 'Stream Prop', 'Stream' is 'FEED', 'Prop Set' is 'HOCEDESIGN THERMAL THERM THERM VISC VISC', and 'Units' is 'lbm/ft-hr'.

Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface with the 'Main FlowSheet' window. The 'Variables' list includes:

Variable	Definition
INCA	Stream Var Stream=OVERHEAD Substream=MIXED Variable=MASS-FLOW Units=lb/hr
NICA	Mass Frac Stream=OVERHEAD Substream=MIXED Component=I-C4
XTOL	Mass Frac Stream=BOTTOMS Substream=MIXED Component=TOLUENE
CFLOW	Mass Flow Stream=FEED Substream=MIXED Component=N-C5 Units=lb/hr

The 'Edit selected variable' window is open for 'CFLOW'. The 'Reference' is 'Mass Flow', 'Type' is 'Mass Flow', 'Stream' is 'FEED', 'Substream' is 'MIXED', 'Component' is 'N-C5', and 'Units' is 'lb/hr'.

Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface. In the 'Edit selected variable' dialog, the variable 'RR' is selected. The 'Reference' section is expanded, showing the following details:

Variable	Reference
RR	Type: Block Var
	Block: DISTL
	Variable: RR
	Sentence: RR=0.5

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Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface. In the 'Edit selected variable' dialog, the variable 'COND' is selected. The 'Reference' section is expanded, showing the following details:

Variable	Reference
COND	Type: Block Var
	Block: DISTL
	Variable: COND-DUTY
	Sentence: RESULTS
	Units: Btu/hr

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Examples of Accessing Variables (Cont'd)

Example 8: Access the normal boiling point of component TOLUENE

The screenshot shows the Aspen Plus V8.4 interface. In the 'Edit selected variable' dialog, the variable 'TBTOL' is selected. The 'Reference' section is expanded, showing the following details:

Variable	Reference
TBTOL	Type: Unary-Param
	Variable: TB
	ID1: TOLUENE
	ID2: 1

An arrow points to the 'ID2: 1' field with the text "Data Set # - usually 1".

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Examples of Accessing Variables (Cont'd)

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

The screenshot shows the Aspen Plus V8.4 interface. In the 'Edit selected variable' dialog, the variable 'CPIG3' is selected. The 'Reference' section is expanded, showing the following details:

Variable	Reference
CPIG3	Type: Unary-Var
	Variable: CPIG
	ID1: TOLUENE
	ID2: 1
	Element: 3

An arrow points to the 'Element: 3' field with the text "Accessing the 3rd element of CPIG".

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Ideal Gas Heat Capacity Equation in A+

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

□ For example, C_P^{IG} is the ideal gas heat capacity with 11 elements (coefficients)

$$C_{P_8}^{IG} = C_1 + C_2 T + C_3 T^2 + C_4 T^3 + C_5 T^4 + C_6 T^5 \quad \text{for } C_7 \leq T \leq C_8$$
$$C_{P_8}^{IG} = C_9 + C_{10} T^{C_{11}} \quad \text{for } T < C_7$$

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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 !!!

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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

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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.

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Workshop 3A: VCM Sensitivity Analysis

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

