Process Simulation with ASPEN PLUS

CHE654 Course Notes

Section 6: Design Specifications and

Calculator Blocks

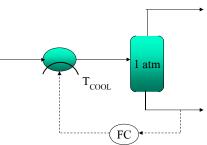
These course materials are applicable to Version 8.4 of ASPEN PLUS ASPEN PLUSTM is a trademark of Aspen Technology, Inc., Burlington, MA, U.S.A.

Setting up a Design Specification Block

- 1. Identify the sampled variables.
- 2. Quantify the goal (objective function).
- 3. Set tolerance.
- 4. Define the manipulated variable.
- 5. Set limits for the manipulated variable.

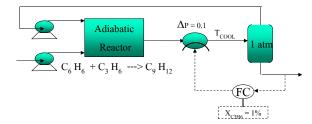
Design Specifications

☐ The design specification (design-spec) feature in A+ can be used to simulate the steady-state performance of a feedback controller.



Design-spec uses the same method of accessing flowsheet variables as in the sensitivity analysis.

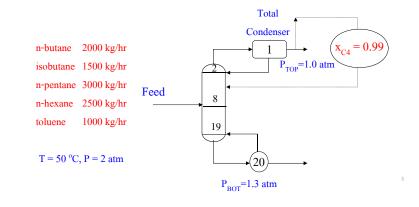
Cumene Production Problem Revisited



- 1. Sampled variable: mole-fraction of C₃H₆ in stream PRODUCT
- 2. Goal: $x_{C3H6} = 0.01$
- 3. Tolerance: 0.0001 (user-defined)
- 4. Manipulated variable: Outlet temperature of the block COOL
- 5. Limits: $50 \le T_{COOL} \le 300^{\circ} C$

Another Example of Design-Spec: DISTL Problem

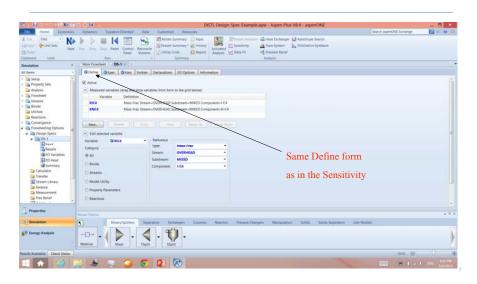
- \Box Recall again the C₄ C₇ separation problem using DISTL
- Set up a Design-Spec to vary the Reflux Ratio (RR) in DISTL so that the mass fraction of C_4 in the overhead is exactly 0.99 (± 0.0001)



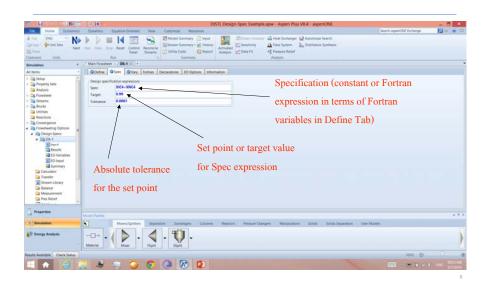
Design-Spec Example (Cont'd)

- Design-Spec feature is invoked by selecting Flowsheeting Options in
 Data pulldown menu.
- ☐ Fill out 1. Define tab => access variables from flowsheet
 - 2. Spec tab => set up an objective function (set point)
 - 3. Vary tab => select a manipulated input variable

Define Tab in Design-Spec



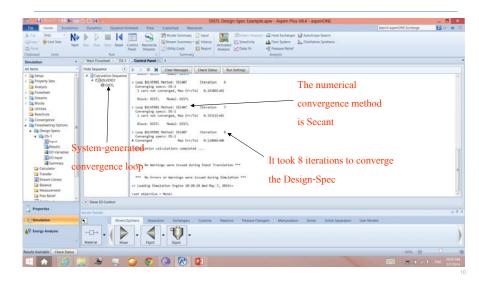
Spec Tab in Design-Spec



Vary Tab in Design-Spec

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Convergence History of the Design-Spec



Viewing Results of the Design-Spec

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Calculator Blocks

□ Allows users to insert Fortran statements or Excel spreadsheets into

flowsheet computations to perform user-defined tasks.

Applications:

- Calculating or setting input variables before they are used (feedforward control)
- Reading input parameters from a file or the terminal
- Writing results to the History file, Report file, the terminal, or any userspecified external file
- Calling external subroutines
- Writing your own user models

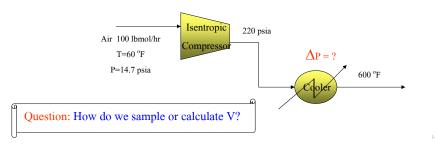
Specifying a Calculator Block

- Define a Calculator block by:
- 1. Creating the Calculator block by selecting Flowsheeting Options in Data pulldown menu
- 2. Identifying the flowsheet variables that the block samples or manipulates.
- 3. Entering the Excel formulas or Fortran statements
- 4. Specifying when the Calculator block is executed

Air Compression & Cooling Problem Revisited

In reality, the pressure drop across the heater block is not zero. It is a function of volumetric flow rate of the inlet stream into the cooler as follows:

$\Delta P = 1.3 \text{ x} 10^{-7} \text{ V}^2$ [=] psia, and V [=] ft³/hr



Define Tab in Calculator

□ Same Define Tab as in Sensitivity and Design-Spec

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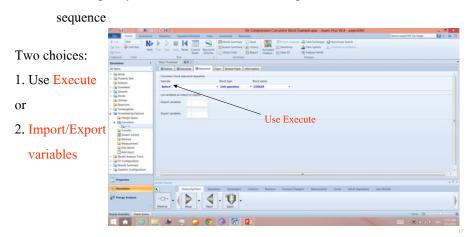
Calculator Tab in Calculator

□ Two calculation methods: Fortran or Excel

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Sequence Tab in Calculator

Used to specify where the calculator block is placed in the execution



Sequence Tab in Calculator (Cont'd)



Either way, we can obtain the same results using Execute and Import/Export Variables

Verifying the Calculated Pressure Drop in COOLER

 \Box V = 6527.141 ft³/hr from base-case simulation

 $\Box \Delta P = 1.3 \times 10^{-7} V^2 = 5.54 psia$

 \Box Outlet P of COOLER = 220 - 5.54 = 214.46 psia

	AIR-FEED	COMP-AIR	COOL-AIR
Temperature F	60.0	870.4	600.0
Pressure psi	14.70	220.00	214.46
Vapor Frac	1.000	1.000	1.000
Mole Flow lbmol/hr	100.000	100.000	100.000
Mass Flow lb/hr	2885.040	2885.040	2885.040
Volume Flow cuft/hr	37928.442	6527.141	5336.987
Enthalpy MMBtu/hr	-0.012	0.572	0.371
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Workshop 3B: VCM Design Specification

 \Box Go to Course Notes Section 9 and work on Workshop 3B.

