Process Simulation with ASPEN PLUS

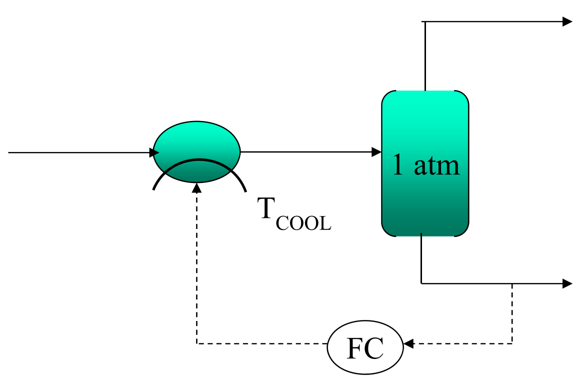
CHE654 Course Notes

Section 6: Design Specifications and Calculator Blocks

These course materials are applicable to Version 8.4 of ASPEN PLUS

Design Specifications

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

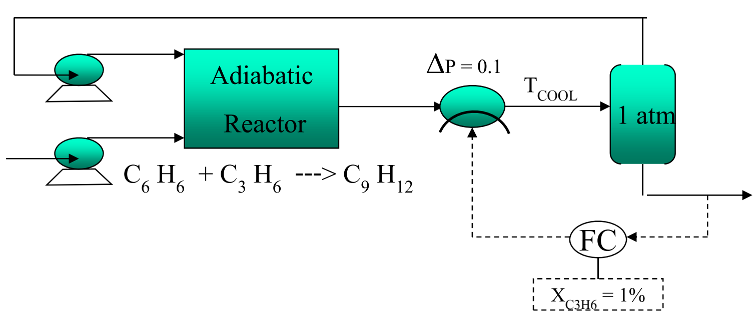


- Design-spec uses the same method of accessing flowsheet variables as in the sensitivity analysis.

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.

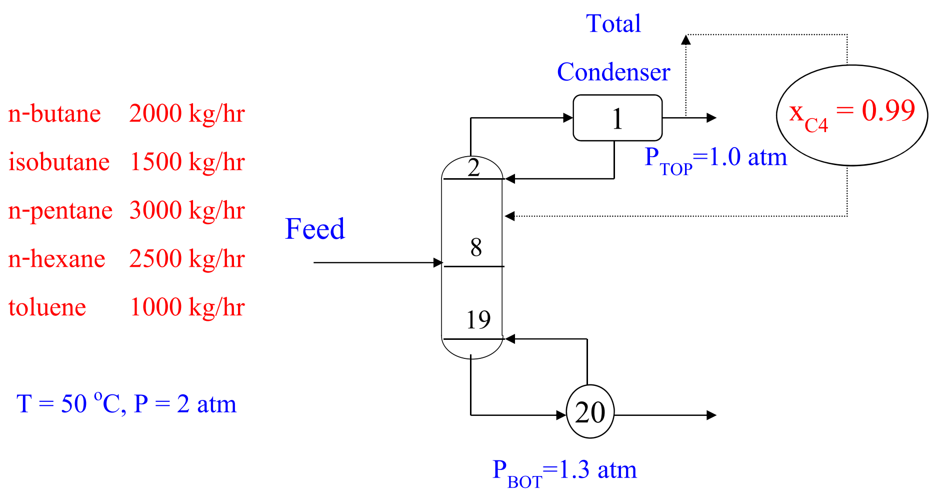
Cumene Production Problem Revisited



1. Sampled variable: mole-fraction of C_3H_6 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: $50 \leq T_{COOL} \leq 300\,^{o}C$

Another Example of Design-Spec: DISTL Problem

- Recall again the C_4 - C_7 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)



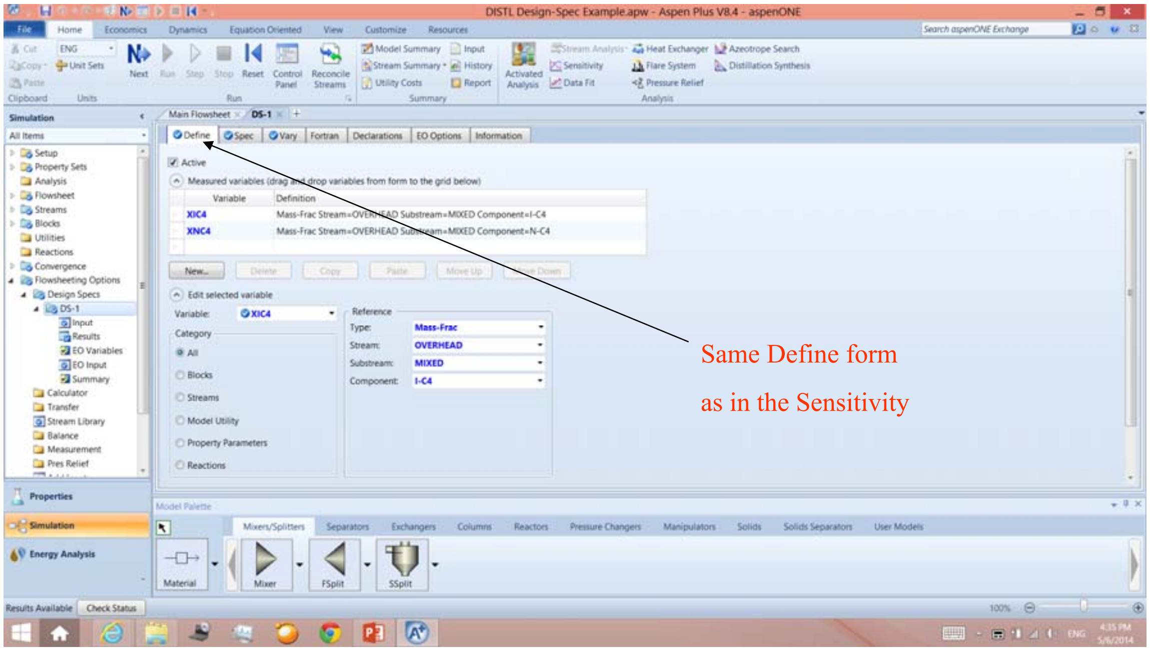
Design-Spec Example (Cont'd)

- Design-Spec feature is invoked by selecting Flowsheeting Options in Data pulldown menu.
- Fill out 1. Define tab => access variables from flowsheet

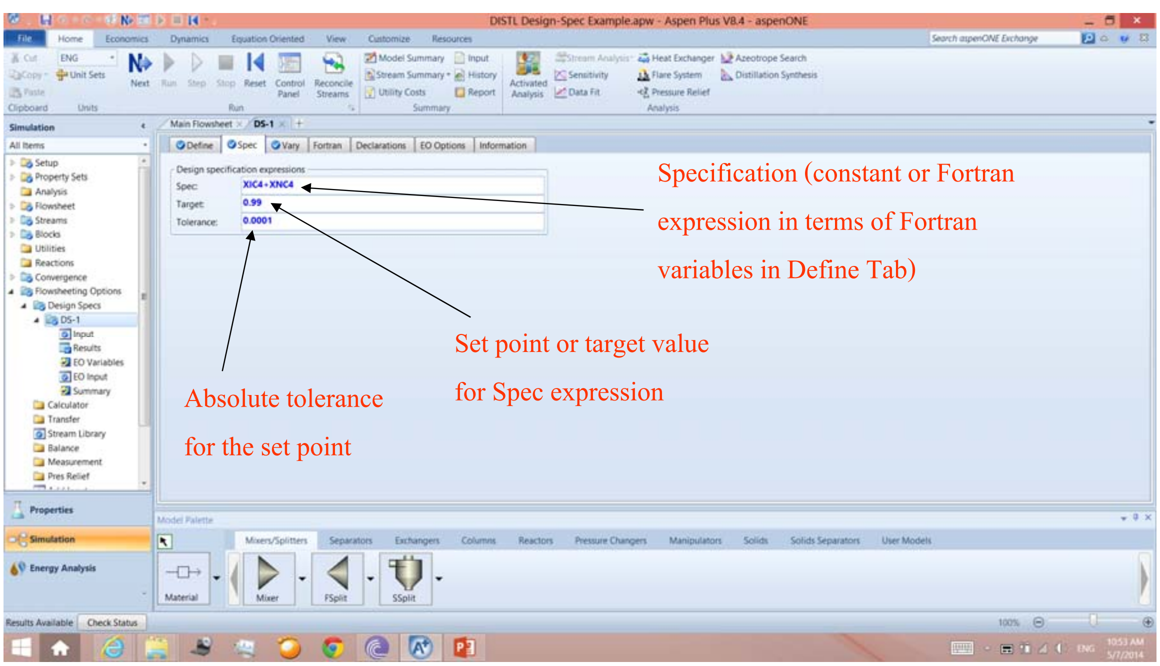
  2. Spec tab => set up an objective function (set point)

  3. Vary tab => select a manipulated input variable

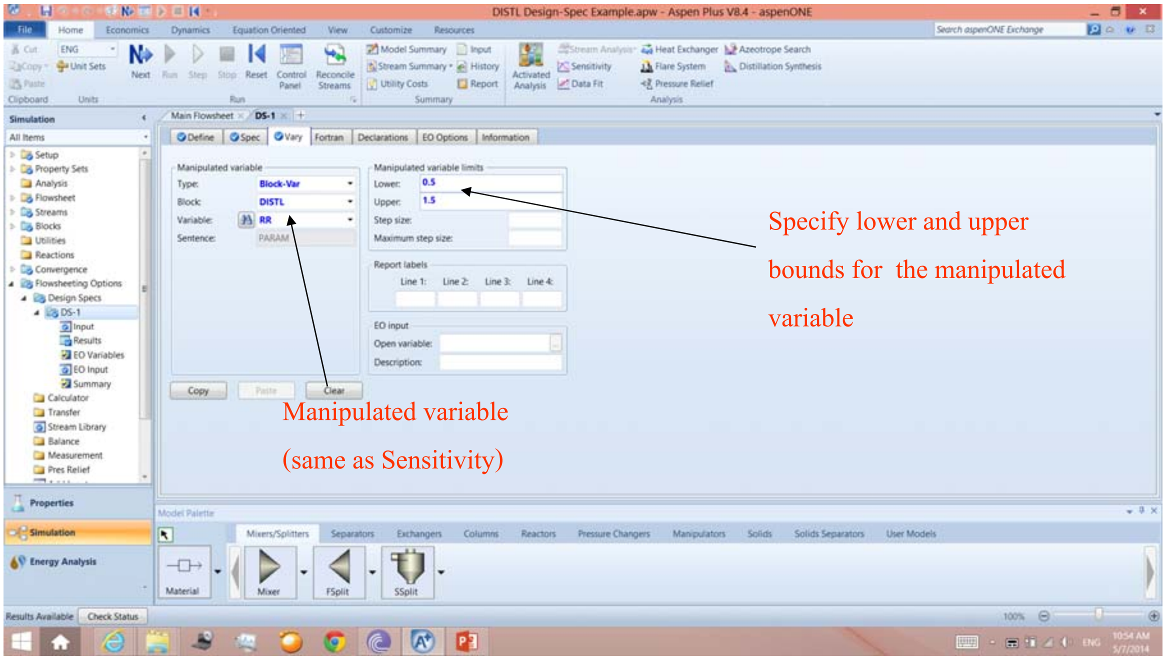
Define Tab in Design-Spec



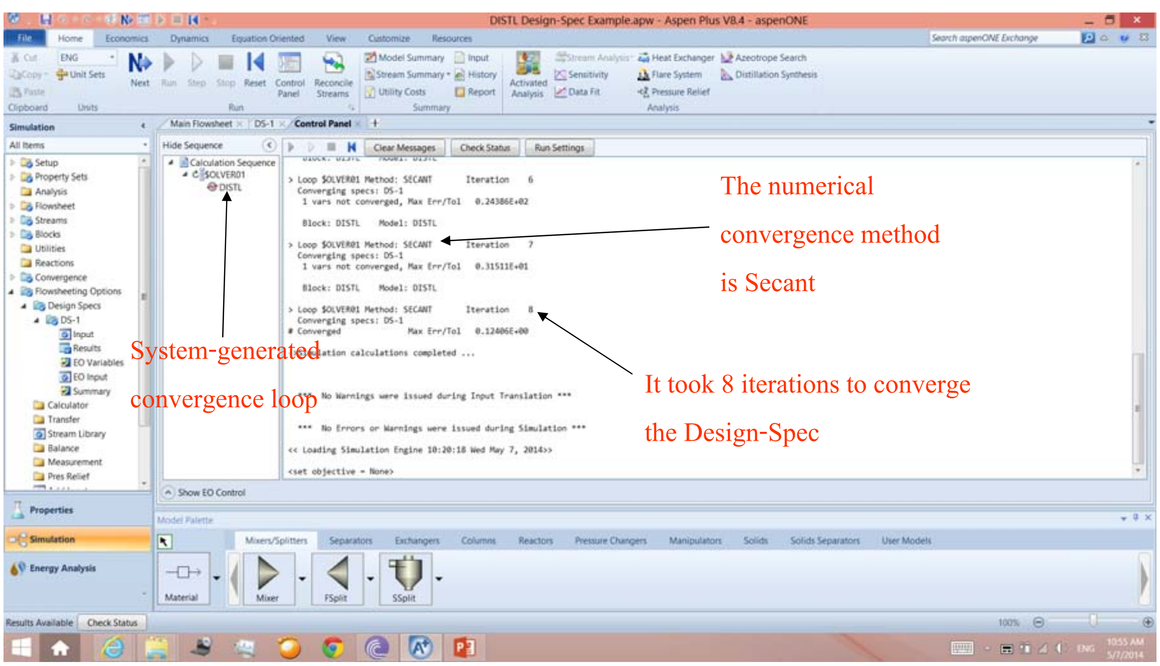
Spec Tab in Design-Spec



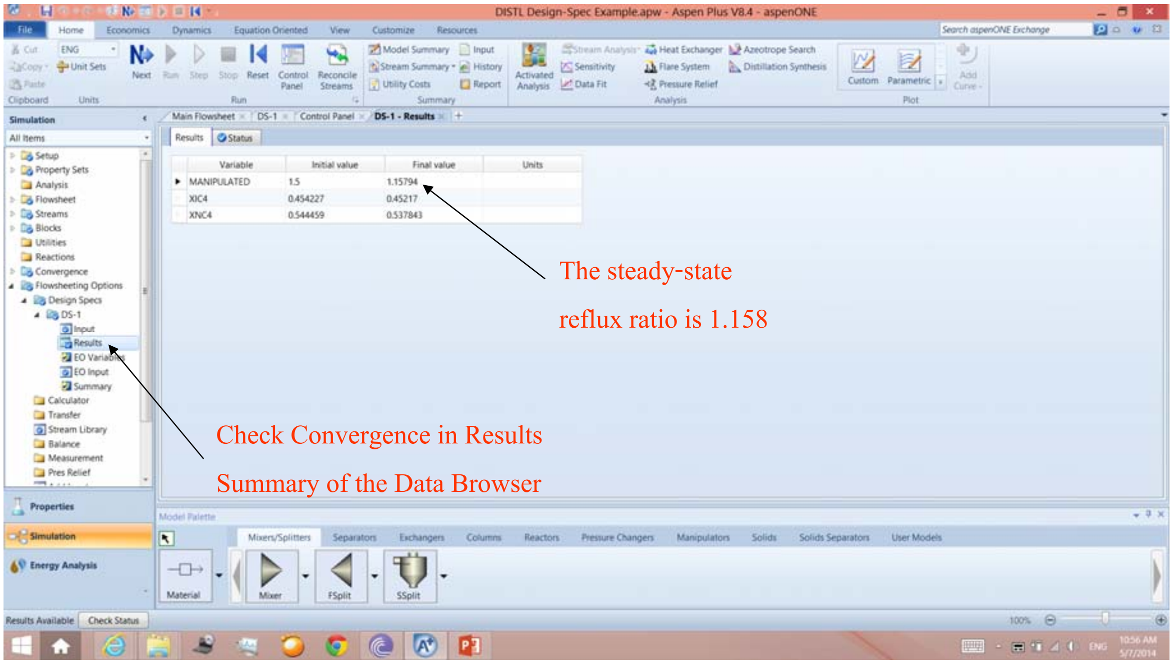
Vary Tab in Design-Spec



Convergence History of the Design-Spec



Viewing Results of the Design-Spec



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 user-specified external file
  - Calling external subroutines
  - Writing your own user models

Specifying a Calculator Block

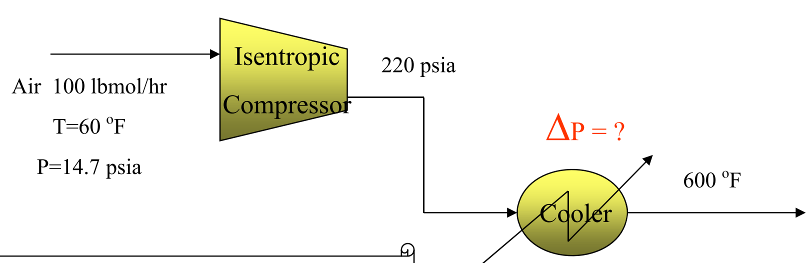
- Define a Calculator block by:

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:

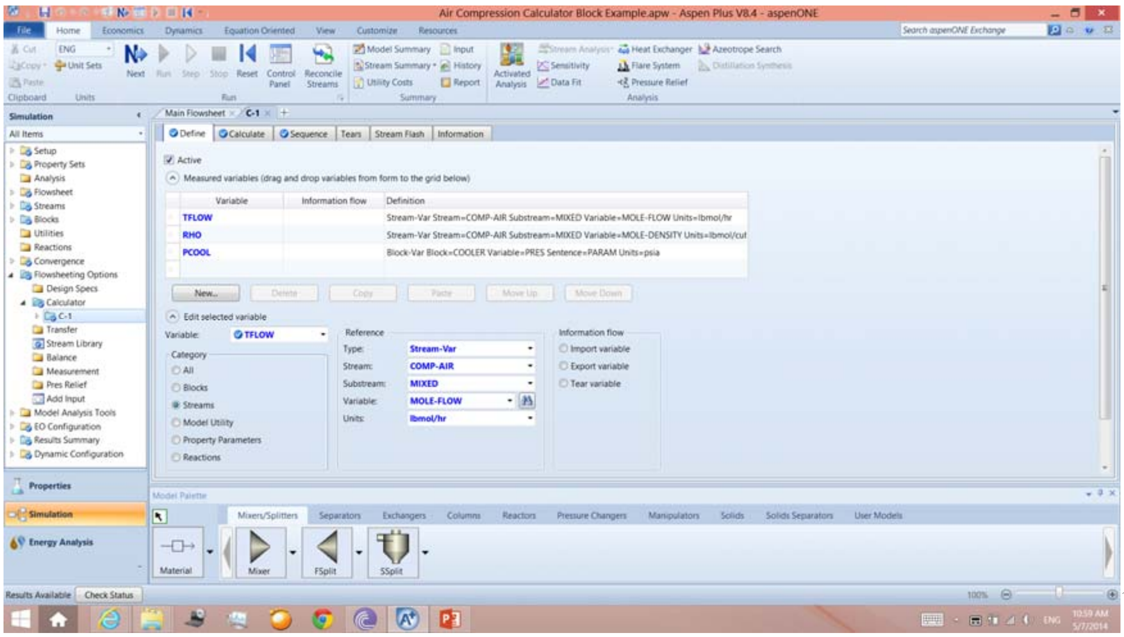
$$\Delta P = 1.3 \times 10^{-7} V^2 \quad [=] \text{ psia, and } V [=] ft^3/hr$$



Question: How do we sample or calculate V?

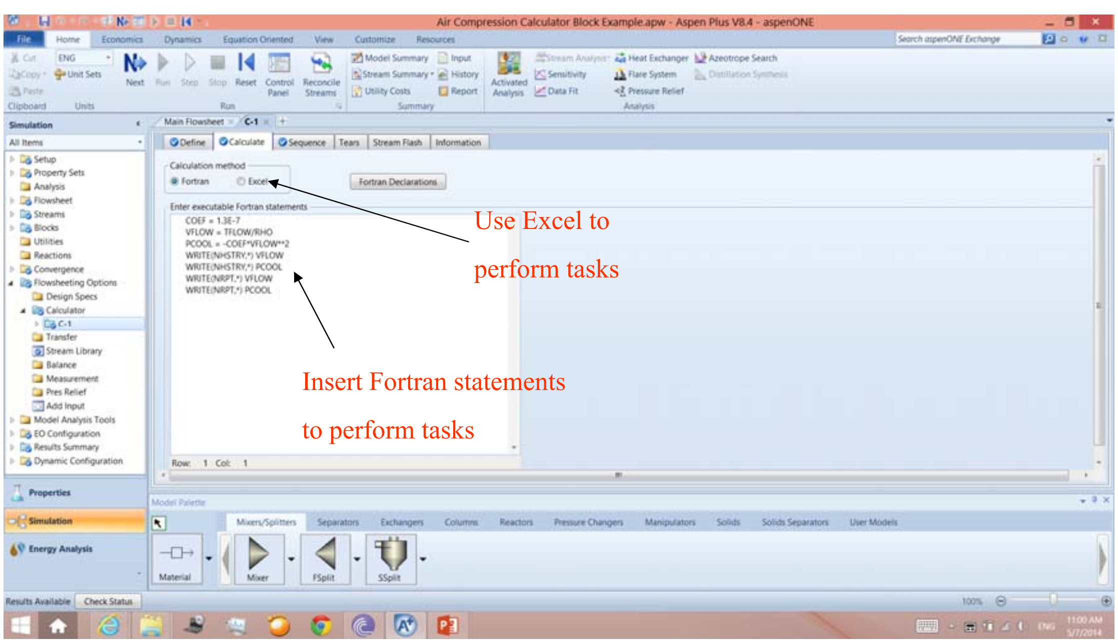
Define Tab in Calculator

- Same Define Tab as in Sensitivity and Design-Spec



Calculator Tab in Calculator

- Two calculation methods: Fortran or Excel



Sequence Tab in Calculator

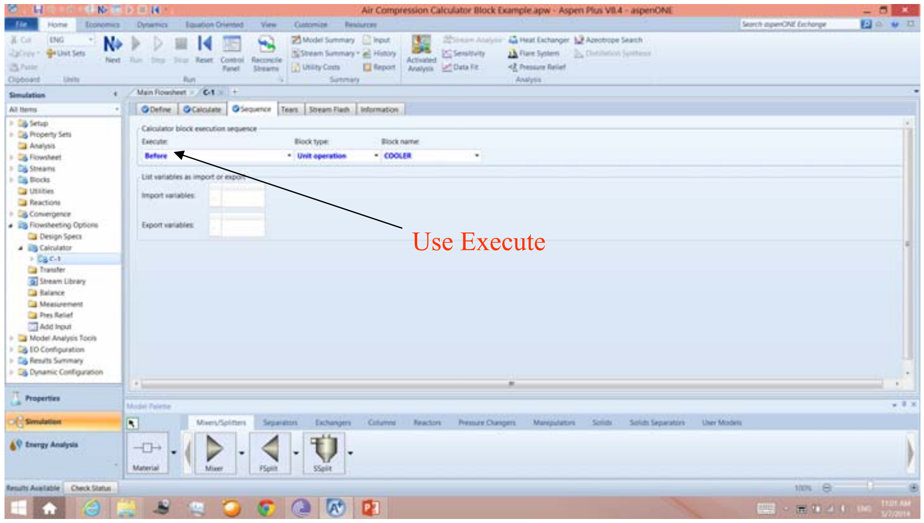
- Used to specify where the calculator block is placed in the execution sequence

Two choices:

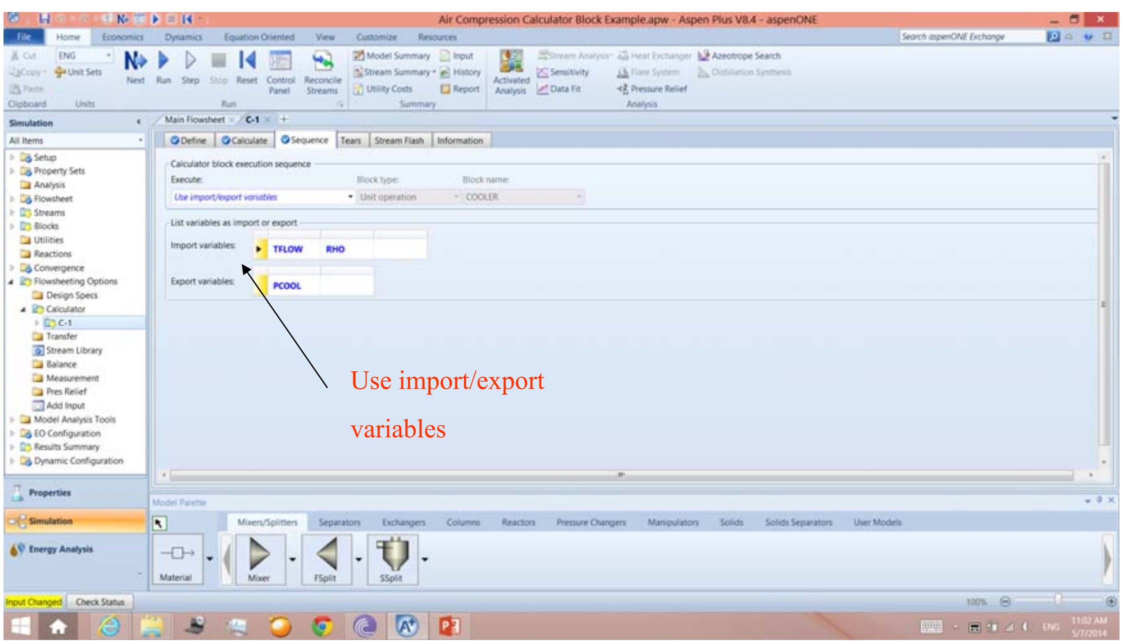
1. Use Execute

or

2. Import/Export variables



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

- V = 6527.141 ft^3/hr from base-case simulation
- $\Delta P = 1.3 \times 10^{-7} V^2 = 5.54$ psia
- 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
Mole Flow lbmol/hr			
N2	79.000	79.000	79.000
O2	21.000	21.000	21.000

Workshop 3B: VCM Design Specification

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