Process Simulation with ASPEN PLUS

CHE654 Course Notes

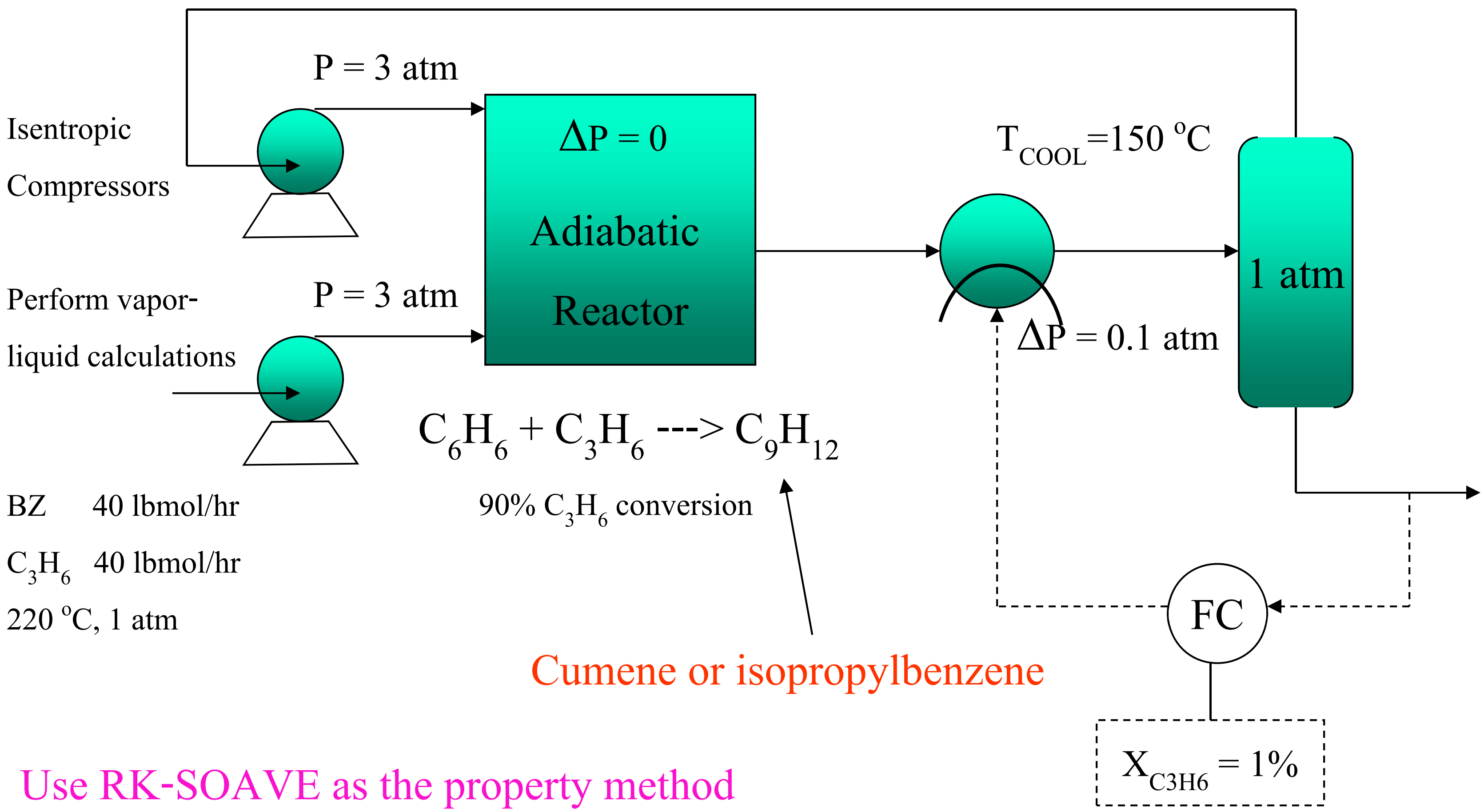
Section 8: Flowsheet Convergence

These course materials are applicable to Version 8.4 of ASPEN PLUS

Flowsheet Convergence

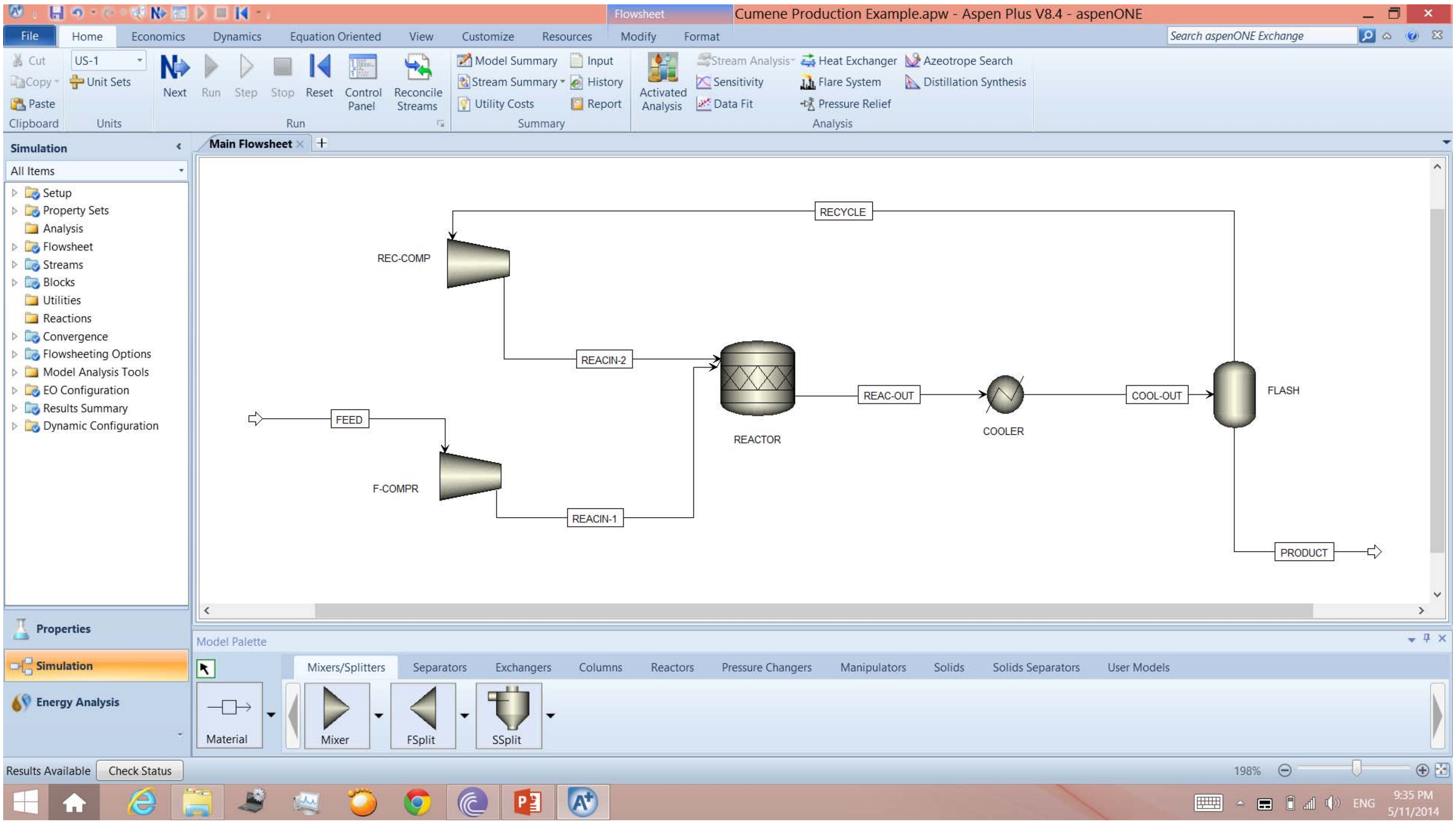
- Convergence arises in flowsheet simulation because ASPEN PLUS is a sequential modular simulator.
- There are 2 kinds of convergence:
  1. Convergence of a recycle stream
  2. Convergence of a design specification
- Know the following terminology :
  - Recycle
  - Design-Spec
  - Tear stream
  - Convergence block

Cumene Production Process Revisited



Use RK-SOAVE as the property method

A+ Flowsheet of the Cumene Production Process



Flowsheet Convergence Specifications

- There are 4 levels of user interaction in specifying the convergence scheme for an A+ simulation run.

- Each subsequent level is more complicated but more flexible than the previous one.

  Level 1: Automatic tearing and sequencing (default)

  – Default convergence methods

  Level 2: Designation of preferred tear streams

  – Level 1 + user specifies desired set of tear streams

  – Still default convergence methods

Flowsheet Convergence Specifications (Cont'd)

Level 3: Specification of the tear stream and design-specs through convergence blocks

- Level 2 + user specifies desired tear streams and convergence methods

Level 4: Specification of partial or total computational sequences

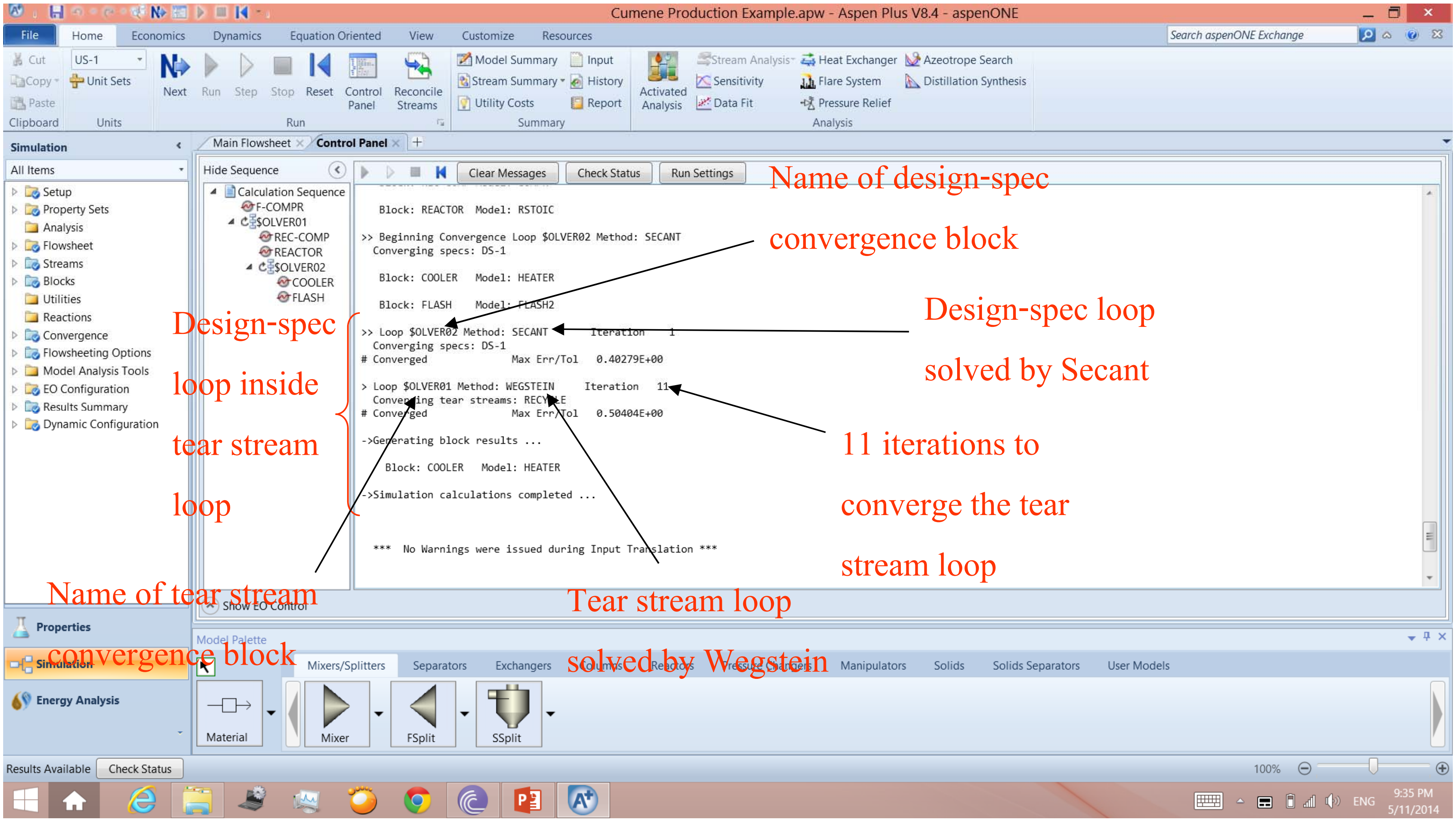
- Level 3 + user specifies a desired partial or complete sequence

Level 1: Automatic Tearing and Sequencing

- A tear set is generated for each MCS* using the method of Motard and Westerberg.
- All tear streams within a MCS are converged simultaneously using the Wegstein method.
- All design-specs are converged individually using the Secant method.
- Design-spec convergence loops are nested inside the tear stream convergence loop.

*** MCS (Maximal Cyclical Subsystem) - a group of blocks which can be converged together.**

Calculation History from Level 1 Convergence



Convergence Methods in A+

- Tear Streams:
  - Wegstein (default)
  - Direct (Successive Substitution)
  - Broyden
  - Newton
- Design Specifications:
  - Secant (default)
  - Broyden
  - Newton

Convergence Results from Level 1

- Computational sequence:

  Block $OLVER01 (Method: WEGSTEIN) has been defined to converge streams: RECYCLE

  Block $OLVER02 (Method: SECANT) has been defined to converge specs: DS-1

  F-COMPR --> $OLVER01 --> REC-COMP --> REACTOR --> $OLVER02 -->

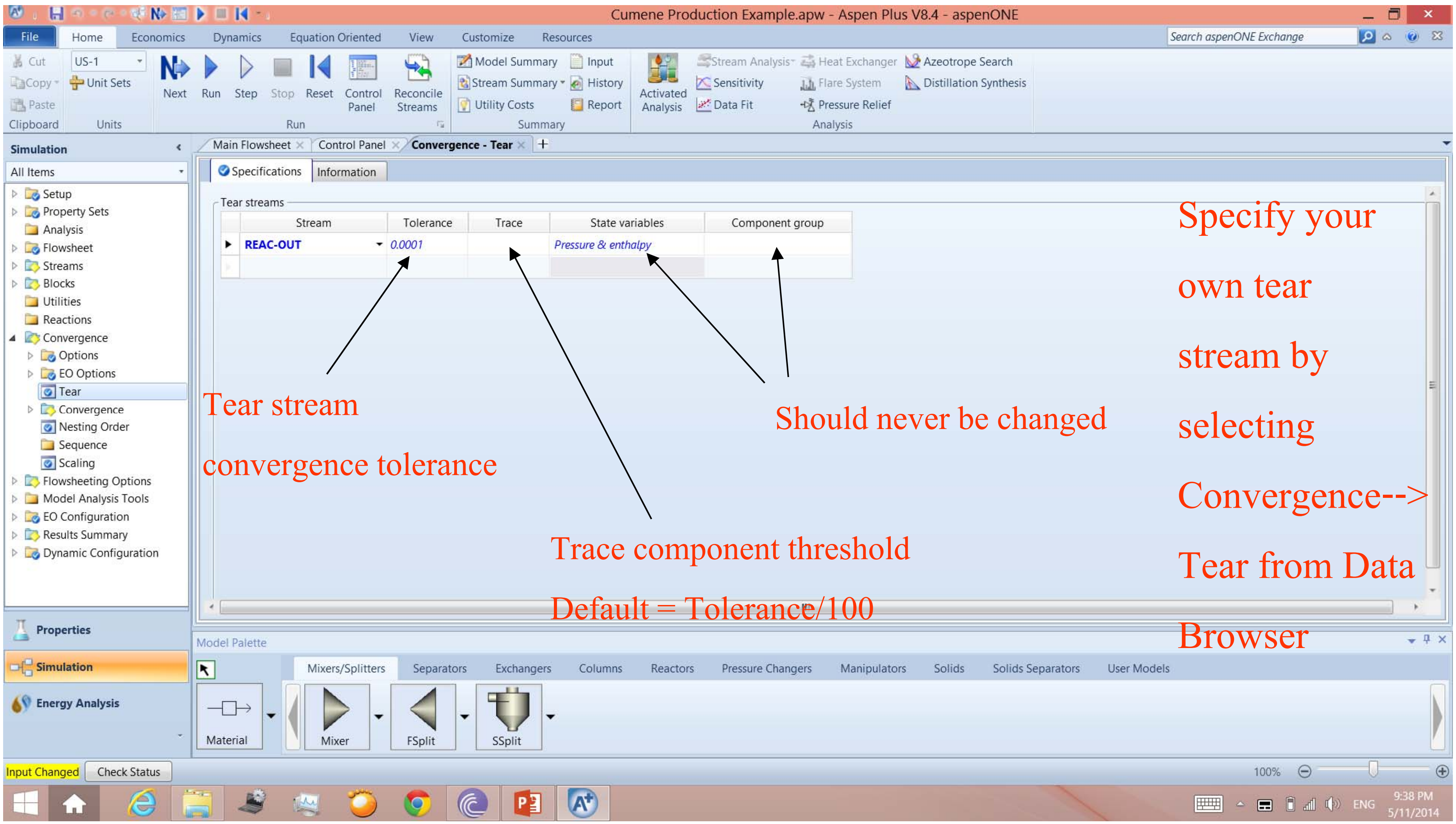
  COOLER --> FLASH --> (RETURN $OLVER02) --> (RETURN $OLVER01)

- What is the calculated T_{COOL} from design-spec? ________________

- What about tear stream? What is the system-generated tear stream?

  ____

Level 2: User-Specified Tear Stream(s)



Level 2: User-Specified Tear Stream(s) (Cont'd)

- Allows users to enter a good initial guess for the desired tear stream

- To enter an initial guess, simply enter the input (such as flows, T and P) into the desired tear stream as if it were a feed stream.

- **Tolerance** is a relative error = $\left| \dfrac{\mathbf{X}_{\mathbf{calculated}} - \mathbf{X}_{\mathbf{assumed}}}{\mathbf{X}_{\mathbf{assumed}}} \right|$

Level 2: User-Specified Tear Stream(s) (Cont'd)

- So what variables in a tear stream are being converged upon?
  - Mole flow of each component, pressure, and mass enthalpy
  - So (N+2) variables, where N is the total number of components
- Convergence criterion:

$$\max_{\text{for all } N+2 \text{ vars}} \left| \frac{X_{cal} - X_{assumed}}{X_{assumed}} \right| \leq 10^{-4}$$

- **Trace** is used to specify the threshold (mole fractions) under which that component would not participate in mass balance.

  Default value = **Tolerance** /100 = 1×10^{-6}

Convergence Results from Level 2

- Computational sequence:

  Block $OLVER01 (Method: WEGSTEIN) has been defined to converge

  streams: REAC-OUT

  Block $OLVER02 (Method: SECANT) has been defined to converge

  specs: DS-1

  F-COMPR --> $OLVER01 --> $OLVER02 --> COOLER --> FLASH -->

  (RETURN $OLVER02) --> REC-COMP --> REACTOR --> (RETURN $OLVER01)

- How many iterations did it take Wegstein to converge the tear stream loop this time? __________________

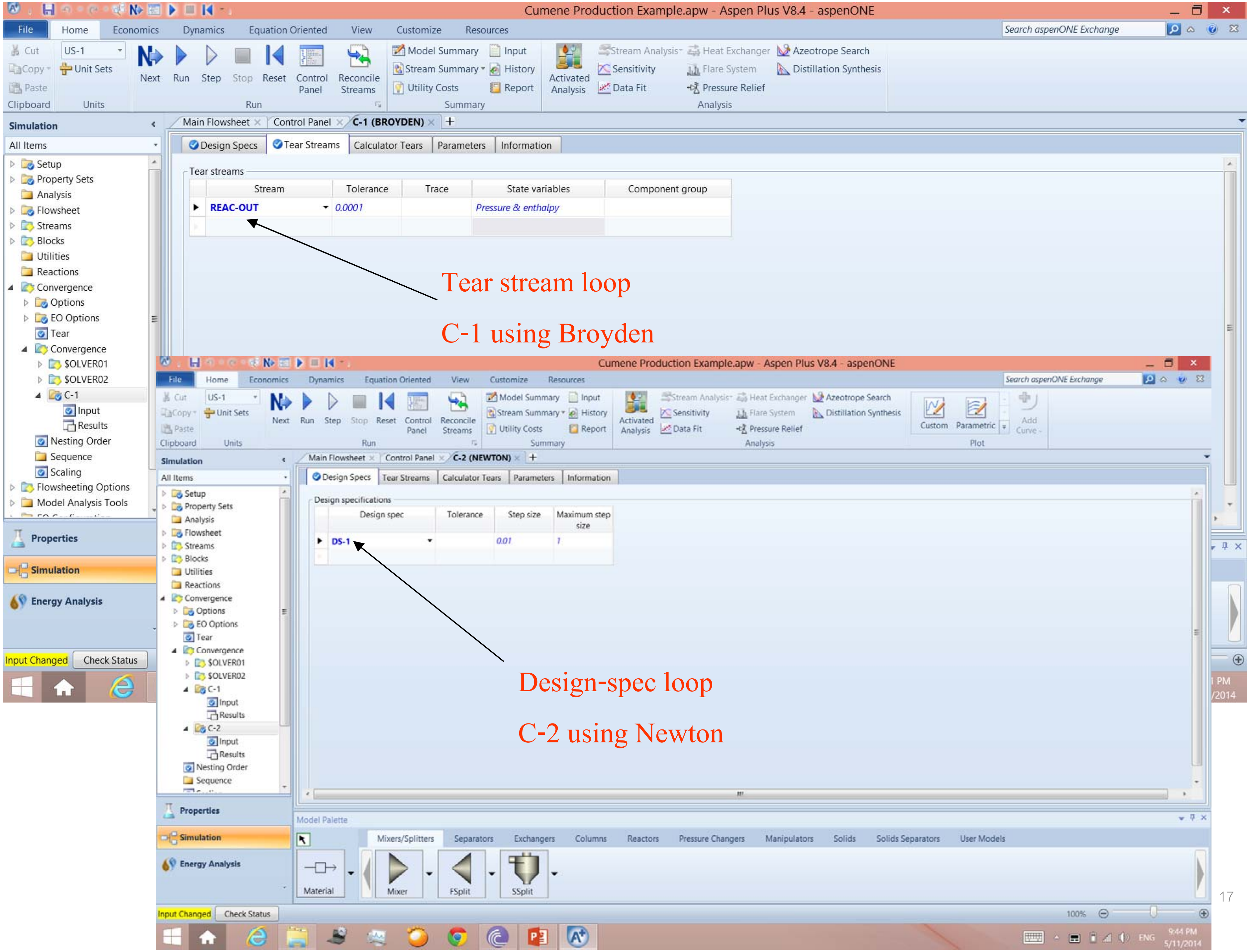
Level 3: User-Specified Convergence Block(s)

- There are 2 benefits in specifying your own convergence block
  - Can choose another numerical method to converge tear streams or design-specs
  - Can choose to converge tear streams and design-specs simultaneously

- We will do 2 things in this exercise:
  1. Choose Broyden to converge the tear stream REAC-OUT, and at the same time choose Newton to converge Design-Spec
  2. Choose Broyden to converge both tear stream and design-spec together

Level 3: Exercise 1

- First reinitialize the run and clear the Convergence Tear Specifications form.
- Create a new convergence block called C-1 for tear stream by selecting Convergence --> Convergence from the Data menu
  - Enter Broyden when asked for convergence Type
  - Specify the desired tear stream in the Tear Streams tab
- Create another convergence block called C-2 for design-spec
  - Enter Newton when asked for convergence Type
  - Specify the design-spec ID in the Design Specs tab


Cumene Production Example.apw - Aspen Plus V8.4 - aspenONE
C-1 (BROYDEN)
Tear Streams
Tear streams
Stream
Tolerance
Trace
State variables
Component group
REAC-OUT
0.0001
Pressure & enthalpy
Tear stream loop
C-1 using Broyden
C-2 (NEWTON)
Design Specs
Design specifications
Design spec
Tolerance
Step size
Maximum step size
DS-1
0.01
1
Design-spec loop
C-2 using Newton

Convergence Results from Level 3: Exercise 1

- Computational sequence:

  F-COMPR --> C-1 --> C-2 --> COOLER --> FLASH --> (RETURN C-2) -->

  REC-COMP --> REACTOR --> (RETURN C-1)

- Note that C-2 is still nested inside C-1 (Design-spec nested inside Tear stream).

- How many iterations did it take Broyden to converge the tear stream loop this time? ___________________

Level 3: Exercise 2 and Results

- Delete C-1 and C-2 convergence blocks in Exercise 1, and reinitialize the run.

- Create a new convergence block called C-1, this time specifying both the Design Specs and the Tear Streams tabs.

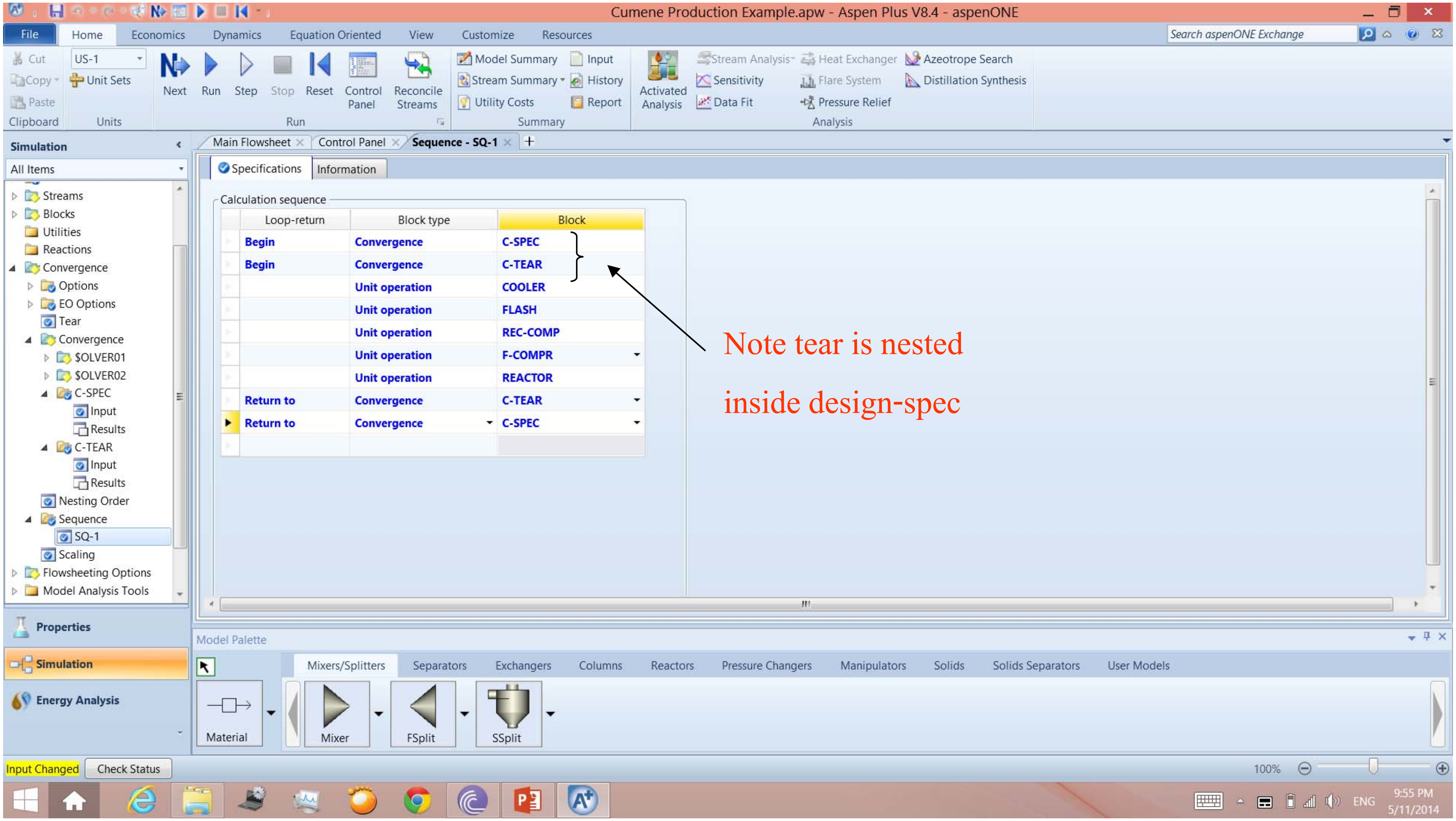
- Computational sequence:

  F-COMPR --> C-1 --> COOLER --> FLASH --> REC-COMP --> REACTOR --> (RETURN C-1)

- How many iterations did it take Broyden to converge both tear stream and design-spec this time? ___________________

Level 4: User-Specified Sequence

- Rarely used
- As an exercise, do the following:
  - Create a convergence block called C-TEAR to converge tear stream REAC-OUT with Broyden.
  - Create a convergence block called C-SPEC to converge the design-spec.
  - Nest C-TEAR inside C-SPEC (opposite of the default in Level 1).
- To specify your own sequence, use Convergence --> Sequence from the Data pulldown menu


Cumene Production Example.apw - Aspen Plus V8.4 - aspenONE
Calculation sequence
Loop-return
Block type
Block
Begin
Convergence
C-SPEC
Begin
Convergence
C-TEAR
Unit operation
COOLER
Unit operation
FLASH
Unit operation
REC-COMP
Unit operation
F-COMPR
Unit operation
REACTOR
Return to
Convergence
C-TEAR
Return to
Convergence
C-SPEC
Note tear is nested
inside design-spec

Convergence Results from Level 4

- Note the following sequence from the Control Panel, which is identical to user-specified C1:

  COMPUTATION ORDER FOR THE FLOWSHEET:

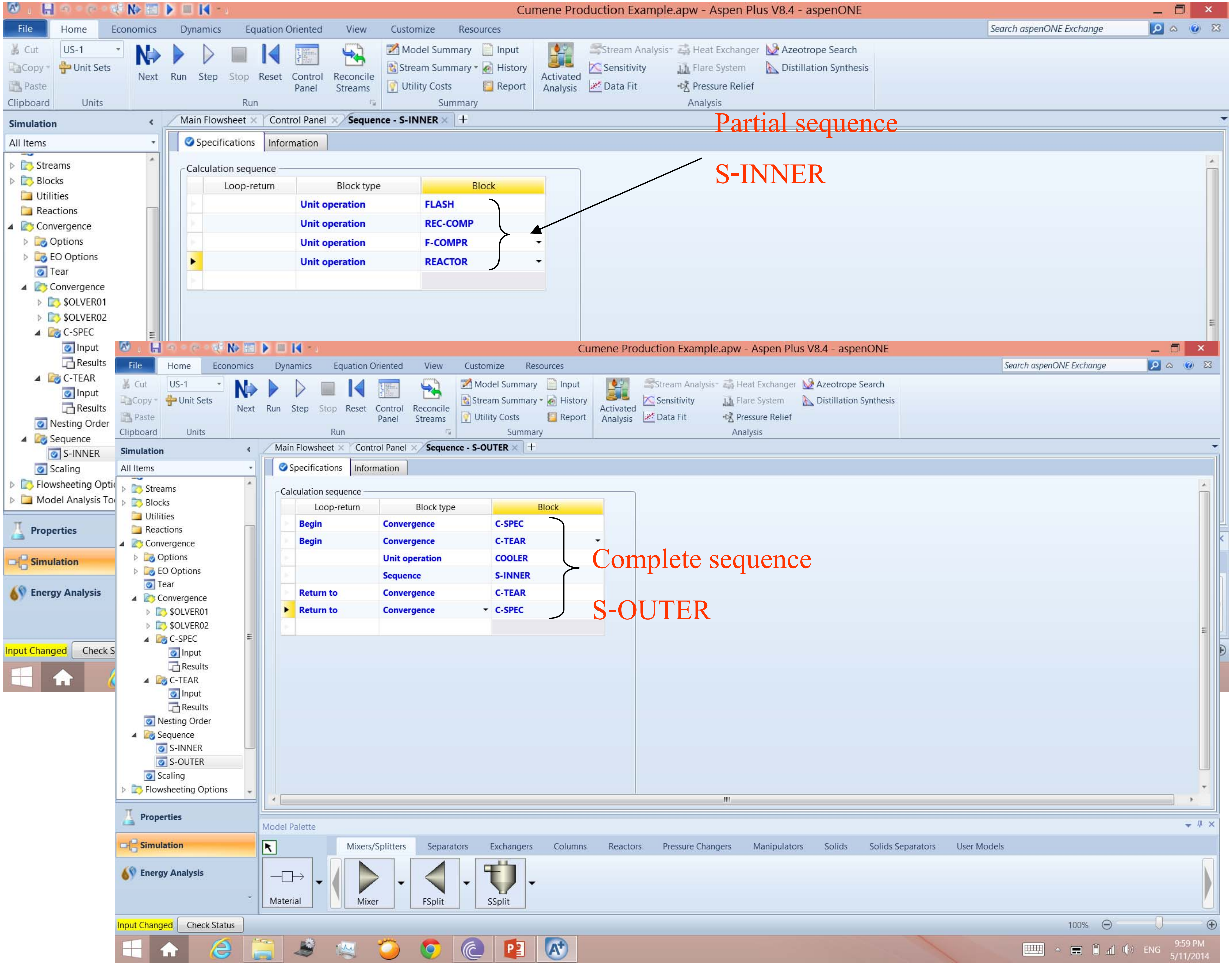
  C-SPEC

  | C-TEAR COOLER FLASH REC-COMP F-COMPR REACTOR

  | (RETURN C-TEAR)

  (RETURN C-SPEC)

- Final note: Partial sequences are allowed.
  - Group blocks FLASH , REC-COMP, F-COMPR, and REACTOR as a partial sequence S- INNER
  - The rest is S-OUTER


Cumene Production Example.apw - Aspen Plus V8.4 - aspenONE
Sequence - S-INNER
Partial sequence
S-INNER
Calculation sequence
Loop-return
Block type
Block
Unit operation
FLASH
Unit operation
REC-COMP
Unit operation
F-COMPR
Unit operation
REACTOR
Sequence - S-OUTER
Begin
Convergence
C-SPEC
Begin
Convergence
C-TEAR
Unit operation
COOLER
Sequence
S-INNER
Return to
Convergence
C-TEAR
Return to
Convergence
C-SPEC
Complete sequence
S-OUTER

Workshop 6: VCM Recycle and Design-Spec Convergence

- For more reading on stream convergence, read the paper

  Don't Let Recycle Stream Stymie Your Simulations by Ryan C. Schad,

  Chemical Engineering Progress, December 1994, pp. 68-76

- Go to Course Notes Section 9 and work on Workshop 6.