

Process Simulation with ASPEN PLUS

CHE654 Course Notes

Section 8: Flowsheet Convergence

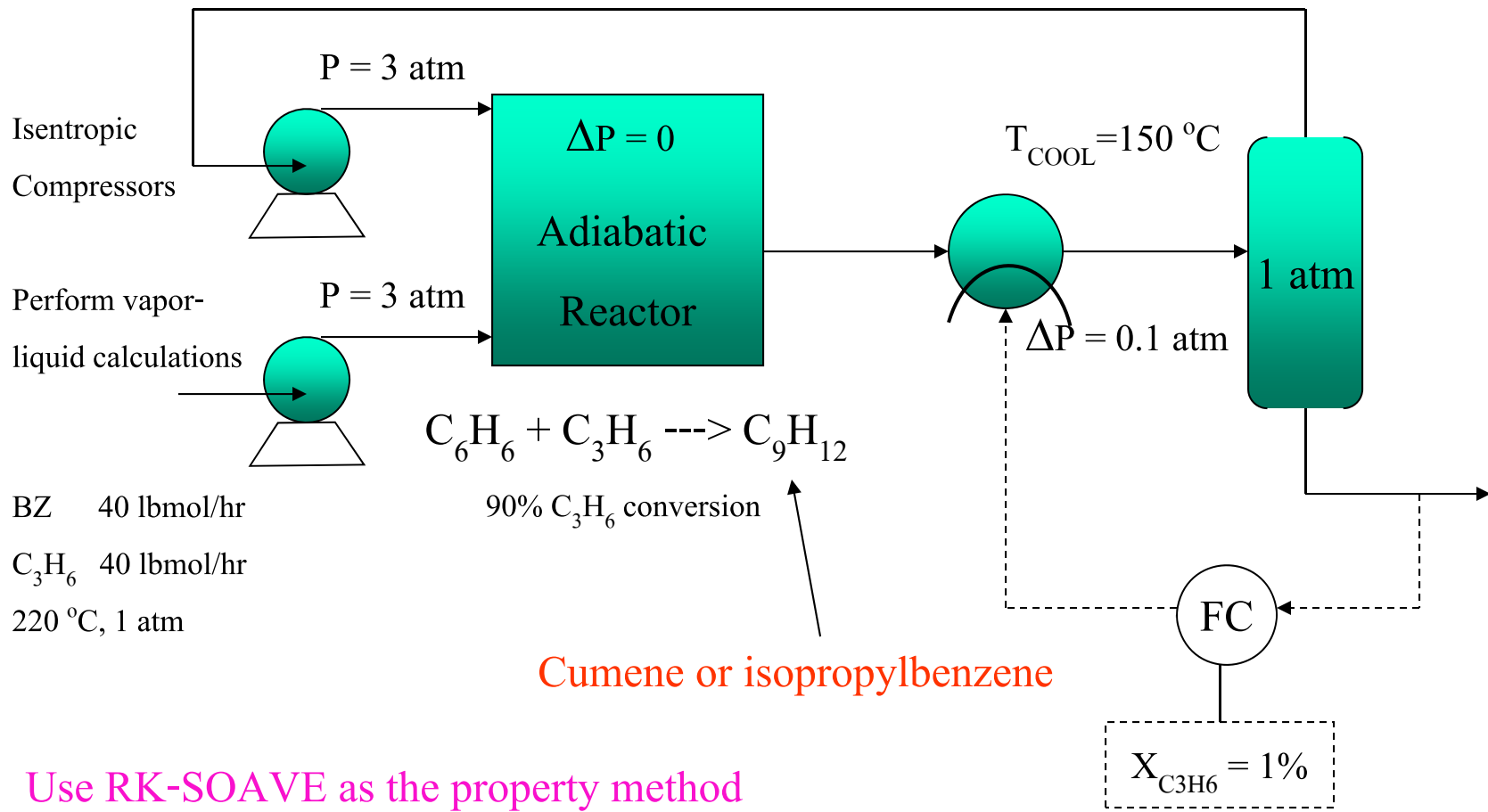
These course materials are applicable to Version 8.4 of ASPEN PLUS

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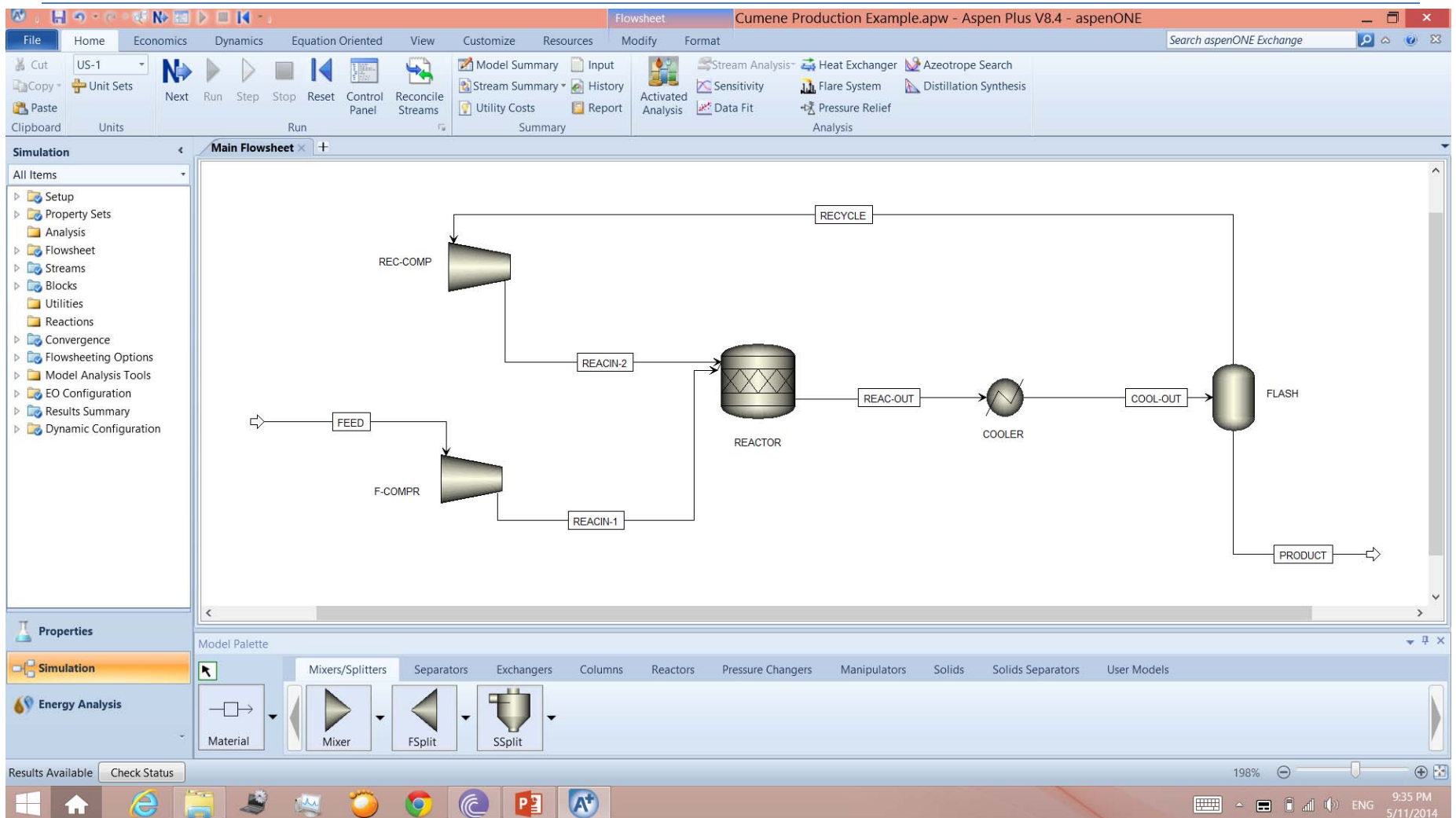
Flowsheet Convergence

- 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



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

The screenshot displays the Aspen Plus V8.4 simulation interface for a 'Cumene Production Example.apw'. The main window shows the 'Control Panel' with a 'Hide Sequence' view. The calculation sequence is as follows:

```

    Calculation Sequence
    └─ F-COMPR
       └─ SOLVER01
          └─ REC-COMP
             └─ REACTOR
                └─ SOLVER02
                   └─ COOLER
                      └─ FLASH

```

The output log in the main window contains the following text:

```

    Block: REACTOR Model: RSTOIC
    >> Beginning Convergence Loop $OLVER02 Method: SECANT
    Converging specs: DS-1
    Block: COOLER Model: HEATER
    Block: FLASH Model: FLASH2
    >> Loop $OLVER02 Method: SECANT Iteration 1
    Converging specs: DS-1
    # Converged Max Err/Tol 0.40279E+00
    > Loop $OLVER01 Method: WEGSTEIN Iteration 11
    Converging tear streams: RECYCLE
    # Converged Max Err/Tol 0.50404E+00
    ->Generating block results ...
    Block: COOLER Model: HEATER
    ->Simulation calculations completed ...
    *** No Warnings were issued during Input Translation ***
  
```

Annotations in red text provide context for the simulation results:

- Name of design-spec convergence block**: Points to the 'DS-1' specification in the SOLVER02 loop.
- Design-spec loop solved by Secant**: Points to the 'Loop \$OLVER02 Method: SECANT' section.
- Design-spec loop inside tear stream loop**: A bracket on the left side groups the SOLVER02 loop and the SOLVER01 loop.
- Name of tear stream convergence block**: Points to the 'RECYCLE' specification in the SOLVER01 loop.
- Tear stream loop solved by Wegstein**: Points to the 'Loop \$OLVER01 Method: WEGSTEIN' section.
- 11 iterations to converge the tear stream loop**: Points to the 'Iteration 11' line in the SOLVER01 loop output.

The interface also shows a 'Properties' pane on the left, a 'Model Palette' at the bottom with 'Mixer', 'FSplit', and 'SSplit' blocks, and a Windows taskbar at the very bottom with the date 5/11/2014 and time 9:35 PM.

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 \$SOLVER01 (Method: WEGSTEIN) has been defined to converge streams: RECYCLE

Block \$SOLVER02 (Method: SECANT) has been defined to converge specs: DS-1

F-COMPR --> \$SOLVER01 --> REC-COMP --> REACTOR --> \$SOLVER02 -->

COOLER --> FLASH --> (RETURN \$SOLVER02) --> (RETURN \$SOLVER01)

□ 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)

The screenshot shows the Aspen Plus V8.4 interface for configuring a tear stream. The 'Convergence - Tear' window is open, displaying a table of tear streams. The 'REAC-OUT' stream is selected, with a tolerance of 0.0001 and state variables of 'Pressure & enthalpy'. Red annotations provide the following information:

- Tear stream convergence tolerance:** Points to the 'Tolerance' column.
- Trace component threshold:** Points to the 'Trace' column.
- Default = Tolerance/100:** A note at the bottom of the window.
- Should never be changed:** Points to the 'State variables' column.
- Specify your own tear stream by selecting Convergence--> Tear from Data Browser:** A vertical note on the right side of the window.

| Stream | Tolerance | Trace | State variables | Component group |
|----------|-----------|-------|---------------------|-----------------|
| REAC-OUT | 0.0001 | | Pressure & enthalpy | |

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 =

$$\frac{X_{\text{calculated}} - X_{\text{assumed}}}{X_{\text{assumed}}}$$

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

□ **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 \$SOLVER01 (Method: WEGSTEIN) has been defined to converge
streams: REAC-OUT

Block \$SOLVER02 (Method: SECANT) has been defined to converge
specs: DS-1

F-COMPR --> \$SOLVER01 --> \$SOLVER02 --> COOLER --> FLASH -->

(RETURN \$SOLVER02) --> REC-COMP --> REACTOR --> (RETURN \$SOLVER01)

- 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

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Model Summary Input Stream Analysis Heat Exchanger Azeotrope Search
Stream Summary History Sensitivity Flare System Distillation Synthesis
Utility Costs Report Activated Analysis Data Fit Pressure Relief Analysis

Simulation Main Flowsheet Control Panel C-1 (BROYDEN)

Design Specs Tear Streams Calculator Tears Parameters Information

| Stream | Tolerance | Trace | State variables | Component group |
|----------|-----------|-------|---------------------|-----------------|
| REAC-OUT | 0.0001 | | Pressure & enthalpy | |

Tear stream loop
C-1 using Broyden

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Model Summary Input Stream Analysis Heat Exchanger Azeotrope Search
Stream Summary History Sensitivity Flare System Distillation Synthesis
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Simulation Main Flowsheet Control Panel C-2 (NEWTON)

Design Specs Tear Streams Calculator Tears Parameters Information

| Design spec | Tolerance | Step size | Maximum step size |
|-------------|-----------|-----------|-------------------|
| DS-1 | | 0.01 | 1 |

Design-spec loop
C-2 using Newton

Model Palette
Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models

Material Mixer FSplit SSplit

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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

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US-1 Unit Sets Next Run Step Stop Reset Control Panel Reconcile Streams

Model Summary Input Stream Analysis Heat Exchanger Azeotrope Search
Stream Summary History Activated Analysis Sensitivity Flare System Distillation Synthesis
Utility Costs Report Summary Data Fit Pressure Relief Analysis

Simulation Main Flowsheet Control Panel Sequence - SQ-1

Specifications Information

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

Model Palette

Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models

Material Mixer FSplit SSplit

Input Changed Check Status

100%

9:55 PM 5/11/2014

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

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Clipboard Units Run Run Step Stop Reset Control Panel Reconcile Streams Summary

Stream Analysis Heat Exchanger Azeotrope Search Sensitivity Flare System Distillation Synthesis Activated Analysis Data Fit Pressure Relief Analysis

Simulation Main Flowsheet Control Panel Sequence - S-INNER

Specifications Information

Calculation sequence

| Loop-return | Block type | Block |
|-------------|----------------|----------|
| | Unit operation | FLASH |
| | Unit operation | REC-COMP |
| | Unit operation | F-COMPR |
| | Unit operation | REACTOR |

Partial sequence
S-INNER

Cumene Production Example.apw - Aspen Plus V8.4 - aspenONE

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Clipboard Units Run Run Step Stop Reset Control Panel Reconcile Streams Summary

Stream Analysis Heat Exchanger Azeotrope Search Sensitivity Flare System Distillation Synthesis Activated Analysis Data Fit Pressure Relief Analysis

Simulation Main Flowsheet Control Panel Sequence - S-OUTER

Specifications Information

Calculation sequence

| Loop-return | Block type | Block |
|-------------|----------------|---------|
| 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

Model Palette

Mixers/Splitters Separators Exchangers Columns Reactors Pressure Changers Manipulators Solids Solids Separators User Models

Material Mixer FSplit SSplit

Input Changed Check Status

100%

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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.

