

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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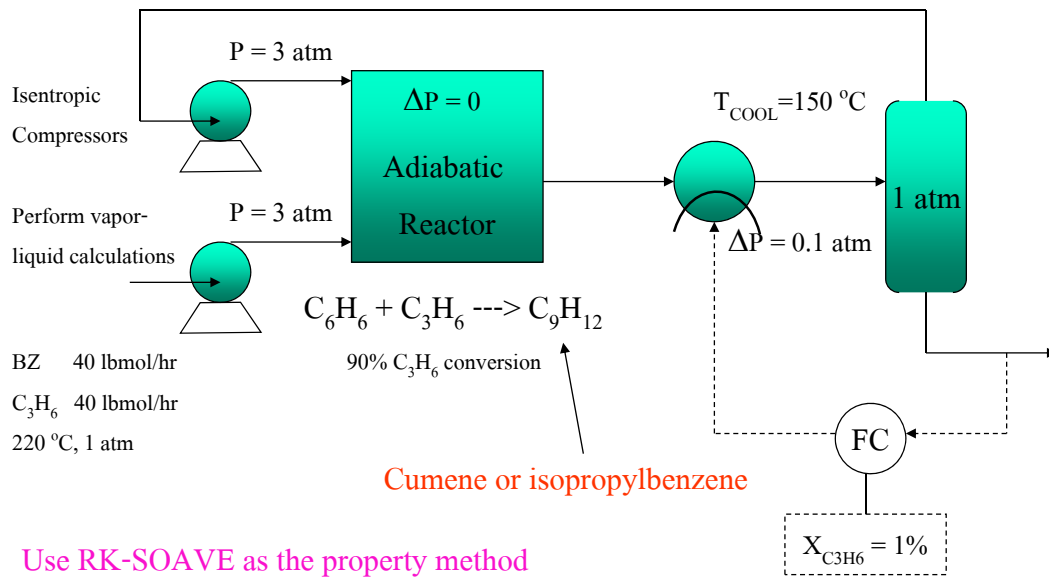
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Flowsheet Convergence

- 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

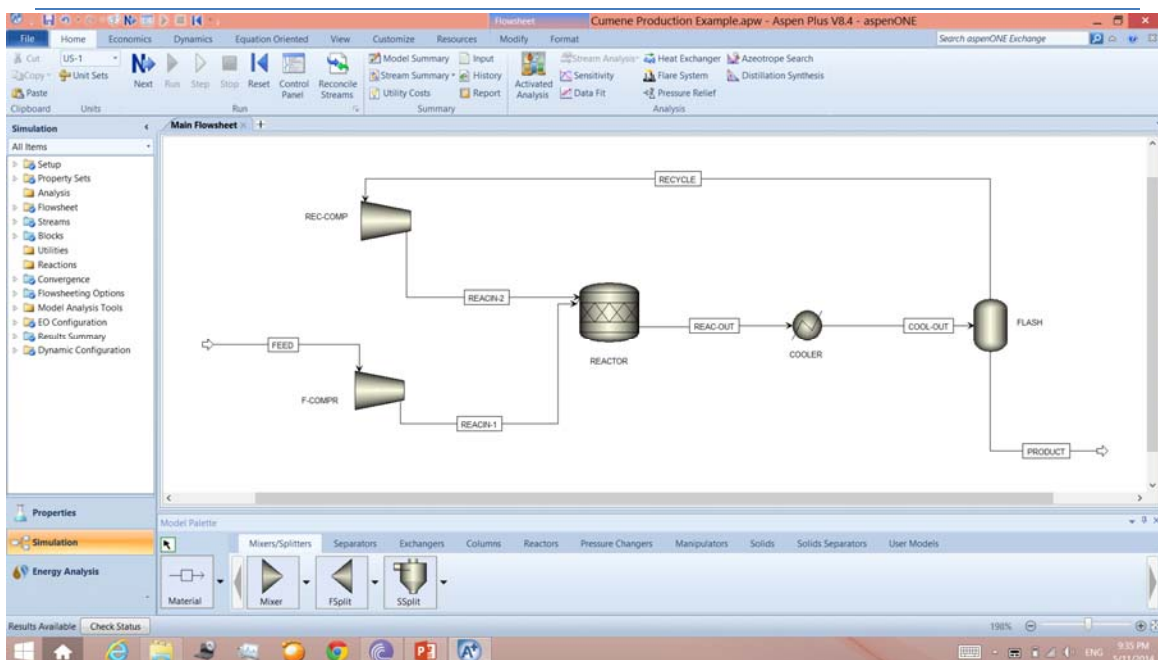
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Cumene Production Process Revisited



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A+ Flowsheet of the Cumene Production Process



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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

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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

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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.

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Calculation History from Level 1 Convergence

The screenshot displays the 'Calculation Sequence' window in Aspen Plus V8.4. The window shows a hierarchical view of the simulation sequence. The 'Design-spec' loop is highlighted in red, showing a 'Loop SOLVER02 Method: SECANT' with 'Converging specs: DS-1'. The 'Tear stream loop' is also highlighted in red, showing a 'Loop SOLVER01 Method: WEGSTEIN' with 'Converging tear streams: REC-COMP'. The simulation history shows that the design-spec loop converged after 11 iterations, and the tear stream loop converged after 11 iterations. The simulation calculations completed successfully.

Annotations in red text point to specific parts of the simulation history:

- Name of design-spec**: Points to 'DS-1' in the 'Converging specs' field.
- convergence block**: Points to the 'Loop SOLVER02 Method: SECANT' block.
- Design-spec loop solved by Secant**: Points to the 'Loop SOLVER02 Method: SECANT' block.
- 11 iterations to converge the tear stream loop**: Points to the 'Iteration 11' line in the 'Loop SOLVER02' block.
- Name of tear stream**: Points to 'REC-COMP' in the 'Converging tear streams' field.
- Tear stream loop solved by Wegstein**: Points to the 'Loop SOLVER01 Method: WEGSTEIN' block.
- Design-spec loop inside tear stream loop**: A bracket indicates the 'Loop SOLVER02' block is nested within the 'Loop SOLVER01' block.

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Convergence Methods in A+

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

- Design Specifications:
 - Secant (default)
 - Broyden
 - Newton

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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?

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Level 2: User-Specified Tear Stream(s)

Specify your own tear stream by selecting Convergence--> Tear from Data Browser

Should never be changed

Trace component threshold
Default = Tolerance/100

Tear stream convergence tolerance

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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 =
$$\left| \frac{X_{\text{calculated}} - X_{\text{assumed}}}{X_{\text{assumed}}} \right|$$

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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}

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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? _____

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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

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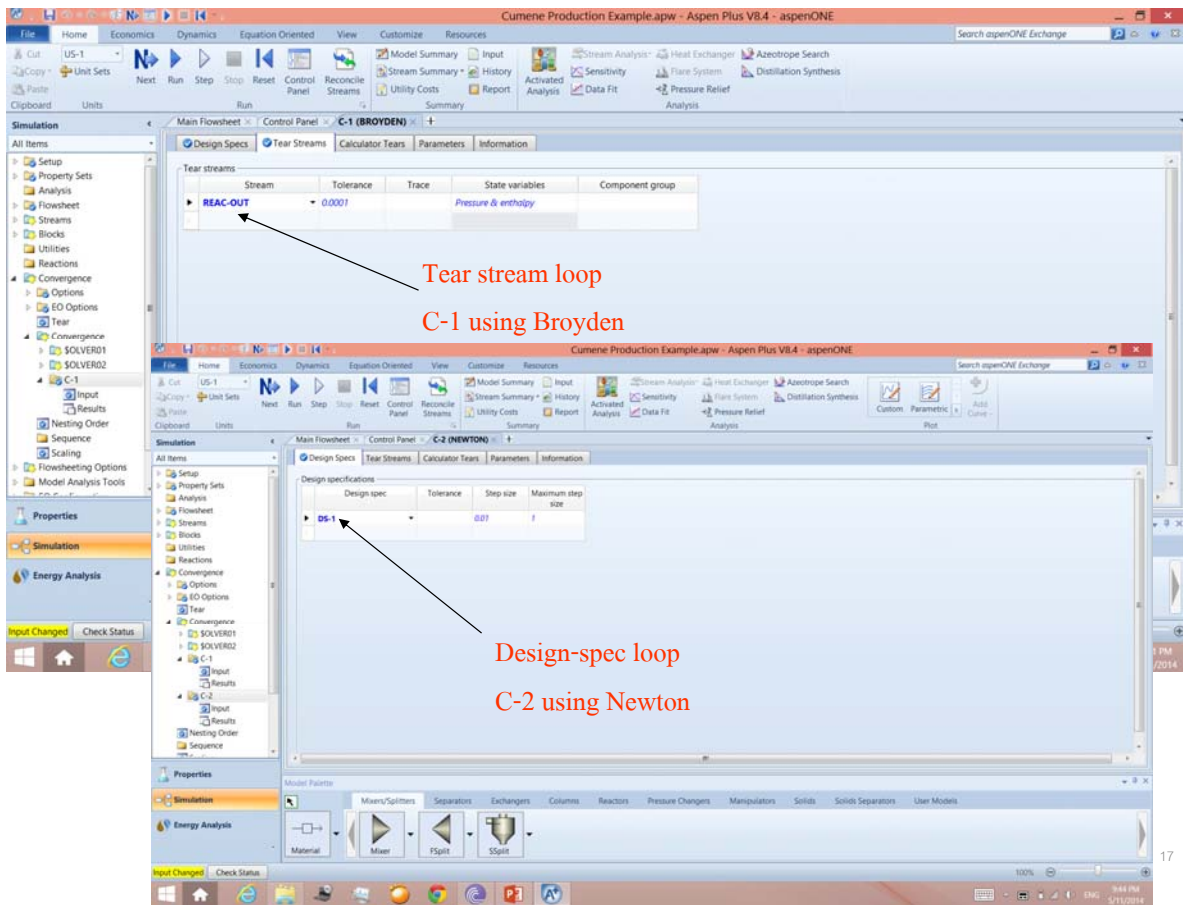
Level 3: Exercise 1

- 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

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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

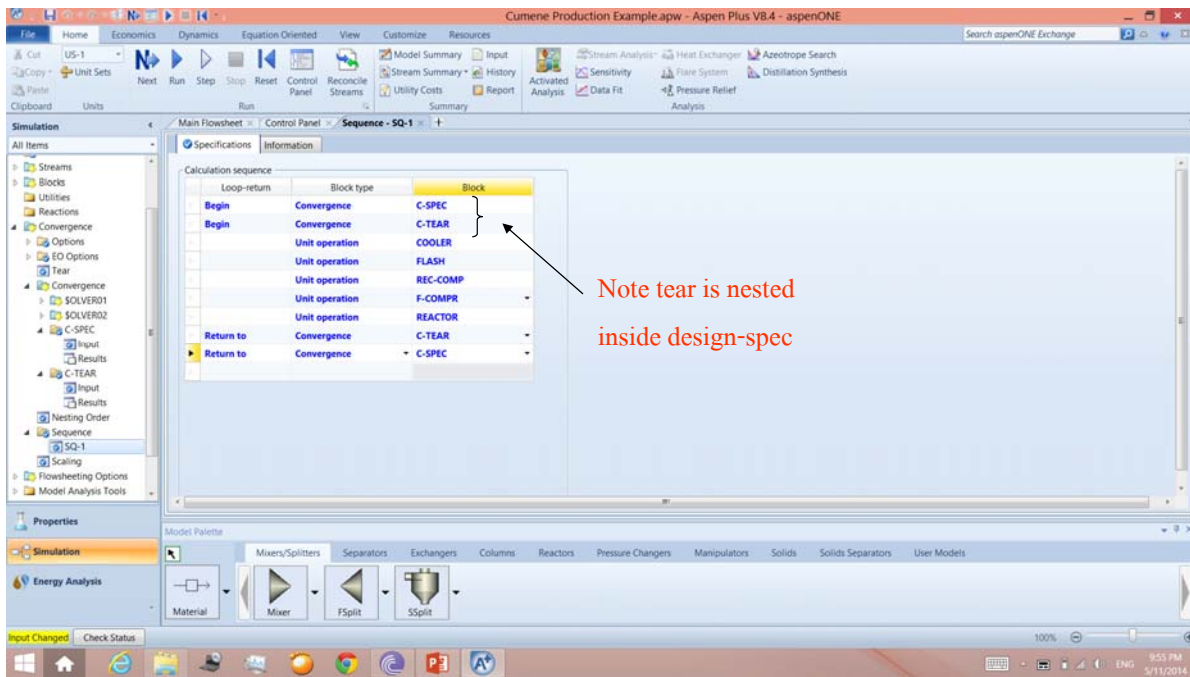
- Delete C-1 and C-2 convergence blocks in Exercise 1, and reinitialize the run.
- Create a new convergence block called C-1, this time specifying both the Design Specs and the Tear Streams tabs.
- **Computational sequence:**
F-COMPR --> C-1 --> COOLER --> FLASH --> REC-COMP --> REACTOR -->
(RETURN C-1)
- How many iterations did it take Broyden to converge both tear stream and design-spec this time? _____

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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

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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

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Partial sequence
S-INNER

Complete sequence
S-OUTER

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

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

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.

