

CHE654 Course Notes

Section 8: Flowsheet Convergence

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.

Flowsheet Convergence

- Convergence arises in flowsheet simulation because ASPEN PLUS is a sequential modular simulator.
 There are 2 kinds of convergence:

 Convergence of a recycle stream
 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



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

Level 2: User-Specified Tear Stream(s)

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

- \Box 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.

 $\Box \text{ Tolerance is a relative error} = \frac{X_{calculated} - X_{assumed}}{X_{assumed}}$

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 for all N+2 vars $\begin{vmatrix} \mathbf{X}_{cal} - \mathbf{X}_{assumed} \\ \mathbf{X}_{assumed} \end{vmatrix} \leq 10^{-4}$
- ☐ **Trace** is used to specify the threshold (mole fractions) under which that component would not participate in mass balance.

Default value = **Tolerance** $/100 = 1 \times 10^{-6}$

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
- U 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

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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
- \Box 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)
- **<u>Final note</u>**: Partial sequences are allowed.
 - Group blocks FLASH , REC-COMP, F-COMPR, and REACTOR as a partial sequence S- INNER
 - The rest is S-OUTER

Workshop 6: VCM Recycle and Design-Spec Convergence

 \Box 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

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

