CO-ChemSep

Nonequilibrium Modelling: the CAPE-OPEN Way

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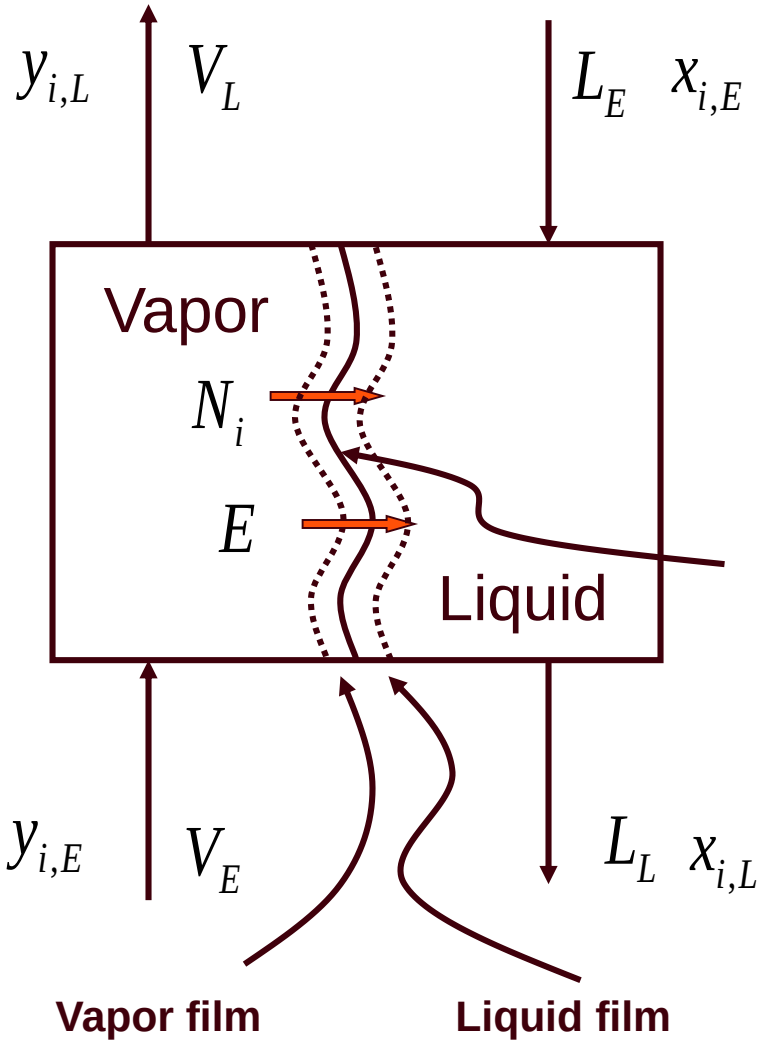
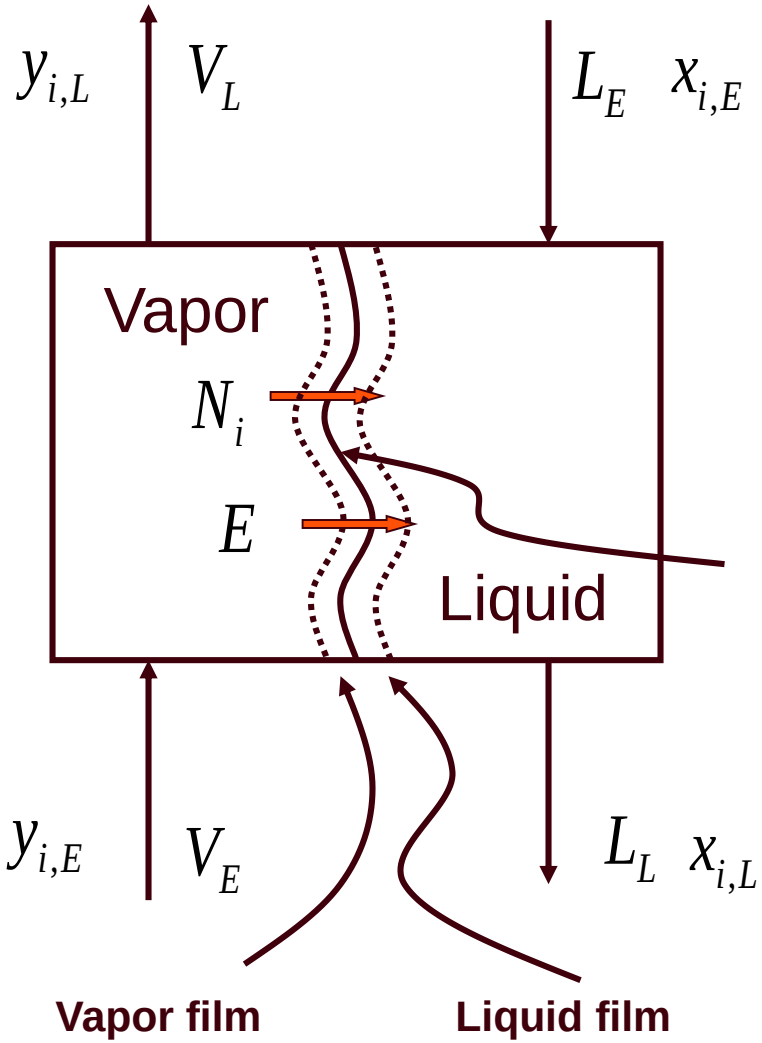
What is ChemSep?

- Just another distillation column simulator.
- Features the original nonequilibrium column model.
- Widely used in academia.
- Few commercial users
  – despite considerable interest.

Nonequilibrium Stage Model





Nonequilibrium Stage Model

Nearly everybody has one!

Aspen Tech
Simulation Sciences ESSCOR
Chemstations
PSE
and many more…

All inspired by the model in ChemSep!

Model Issues:

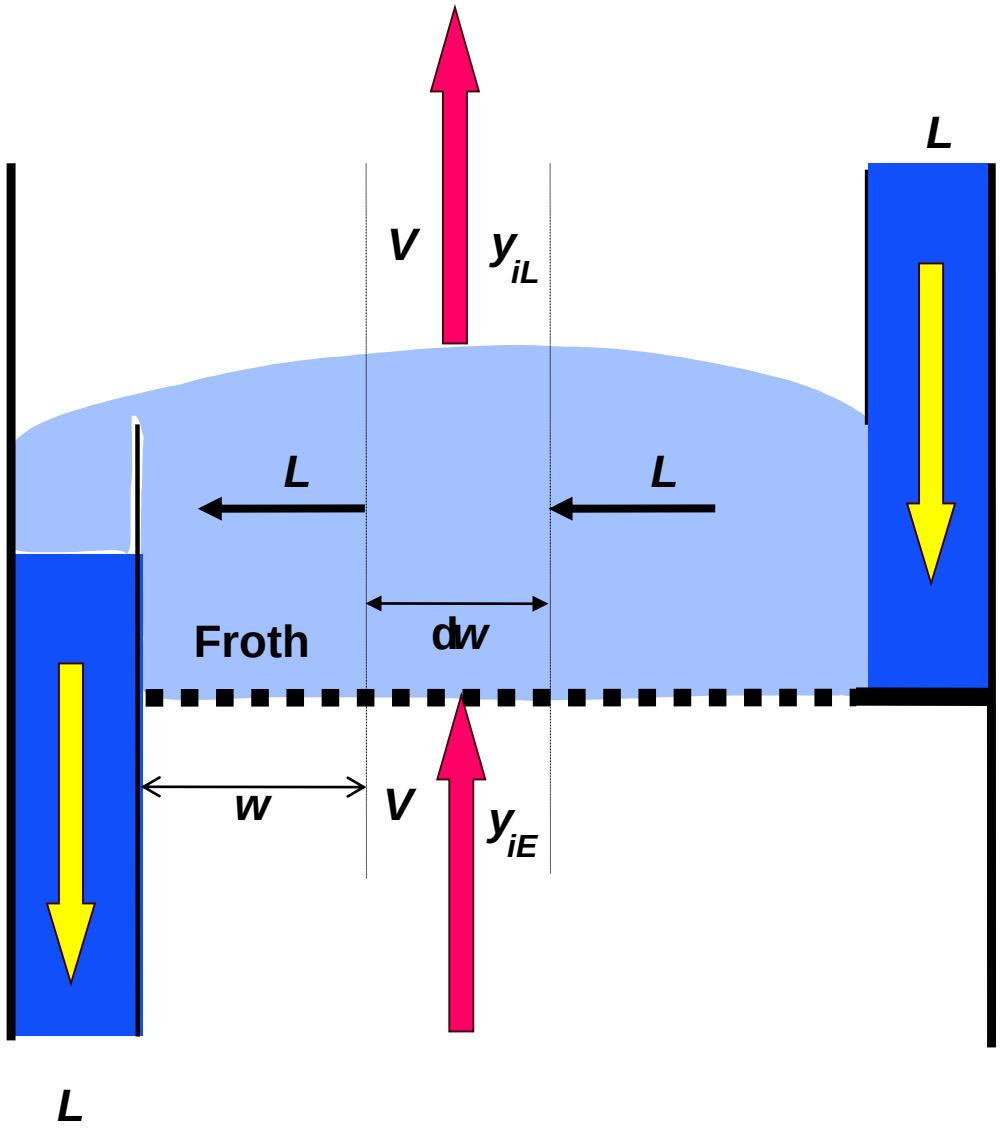
1. Mass transfer coefficients and interfacial areas

   (48 models in ChemSep)
2. Hold up and pressure drop

   (24 models in ChemSep)
3. Flow models

Flow Modeling is Critical!

- Mixed flow
- Plug flow
- Dispersion flow



CO ChemSep: Why?

- Little commercial use
  - despite considerable interest.

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  (because it did not function with flowsheet simulators).

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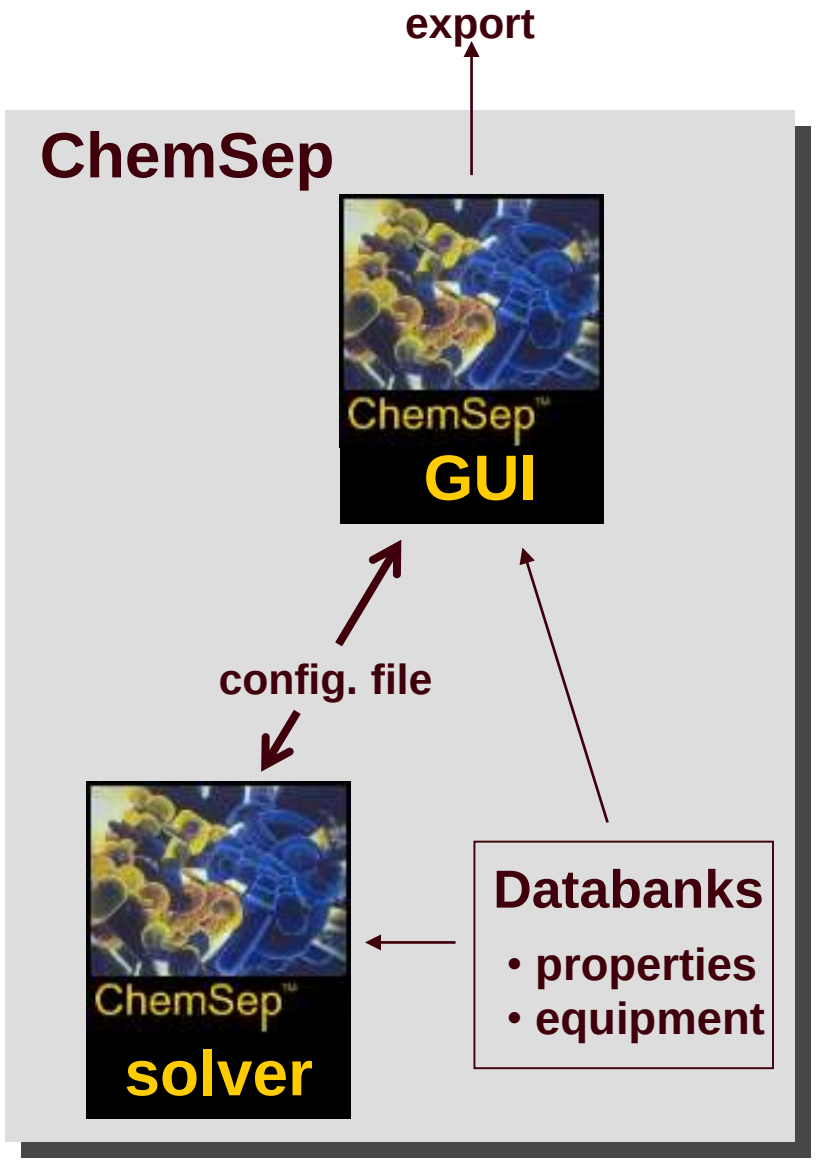
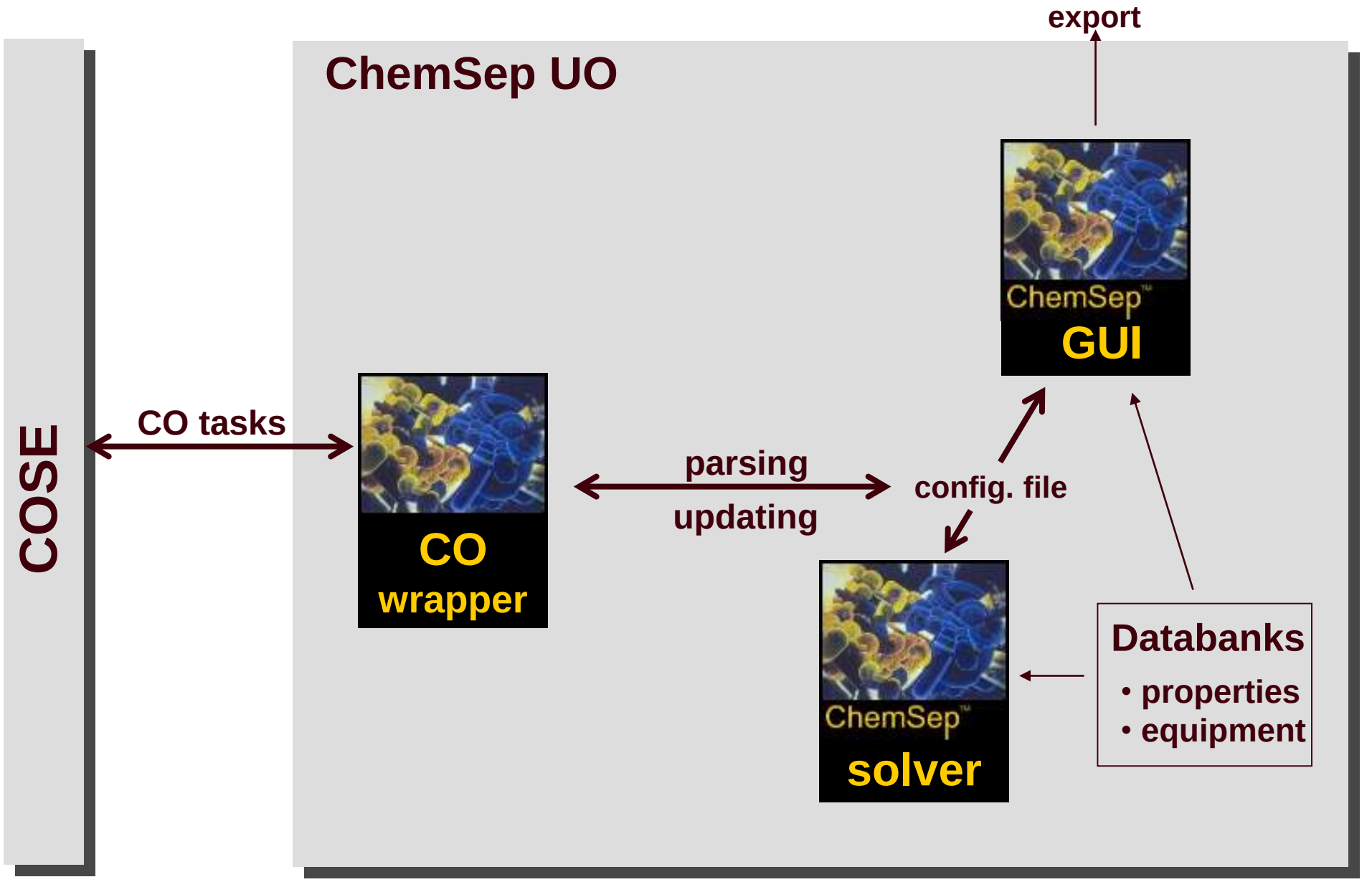
- CAPE-OPEN provides a way to make ChemSep function with any CO process simulator.

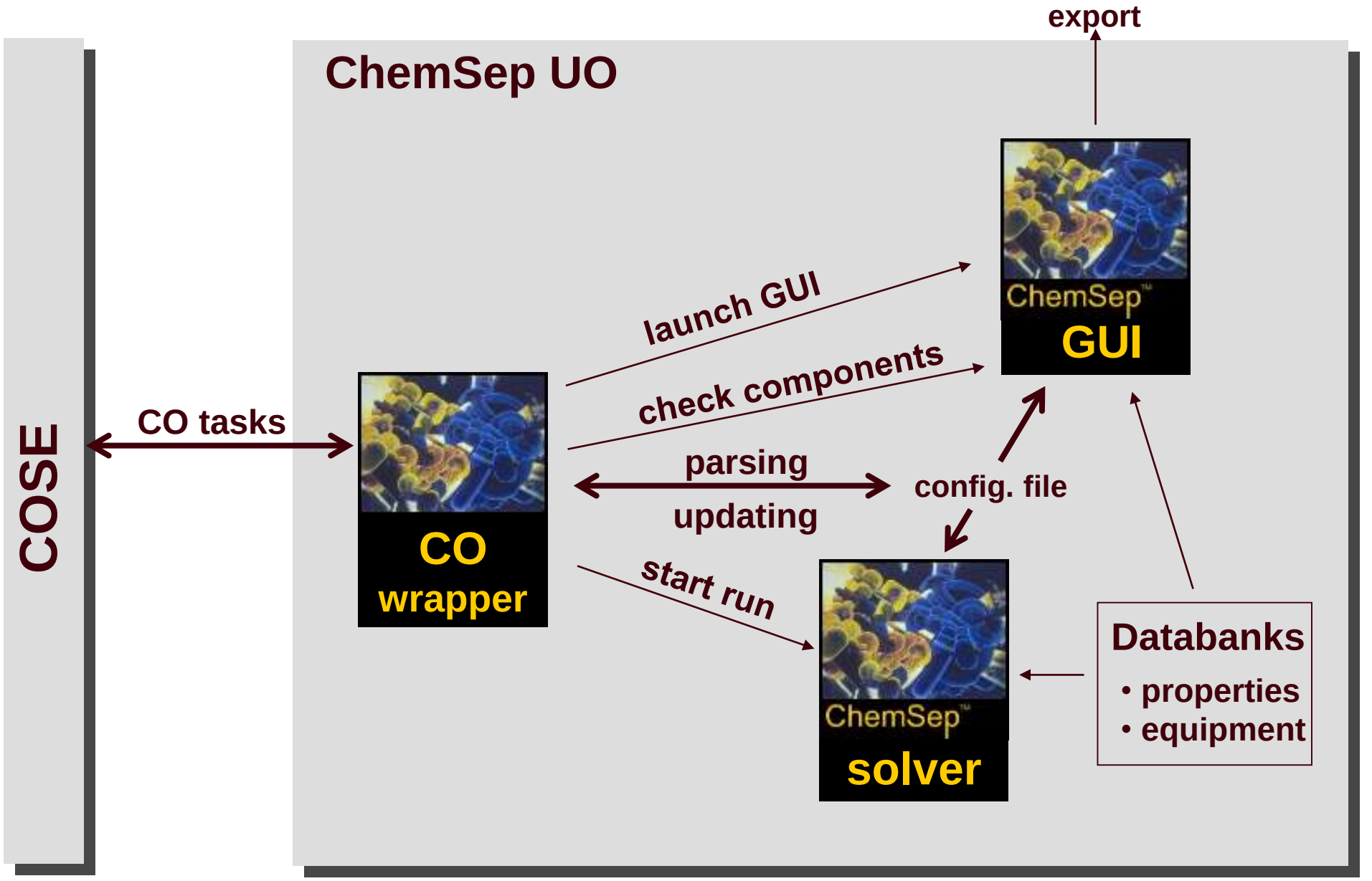
ChemSep Architecture



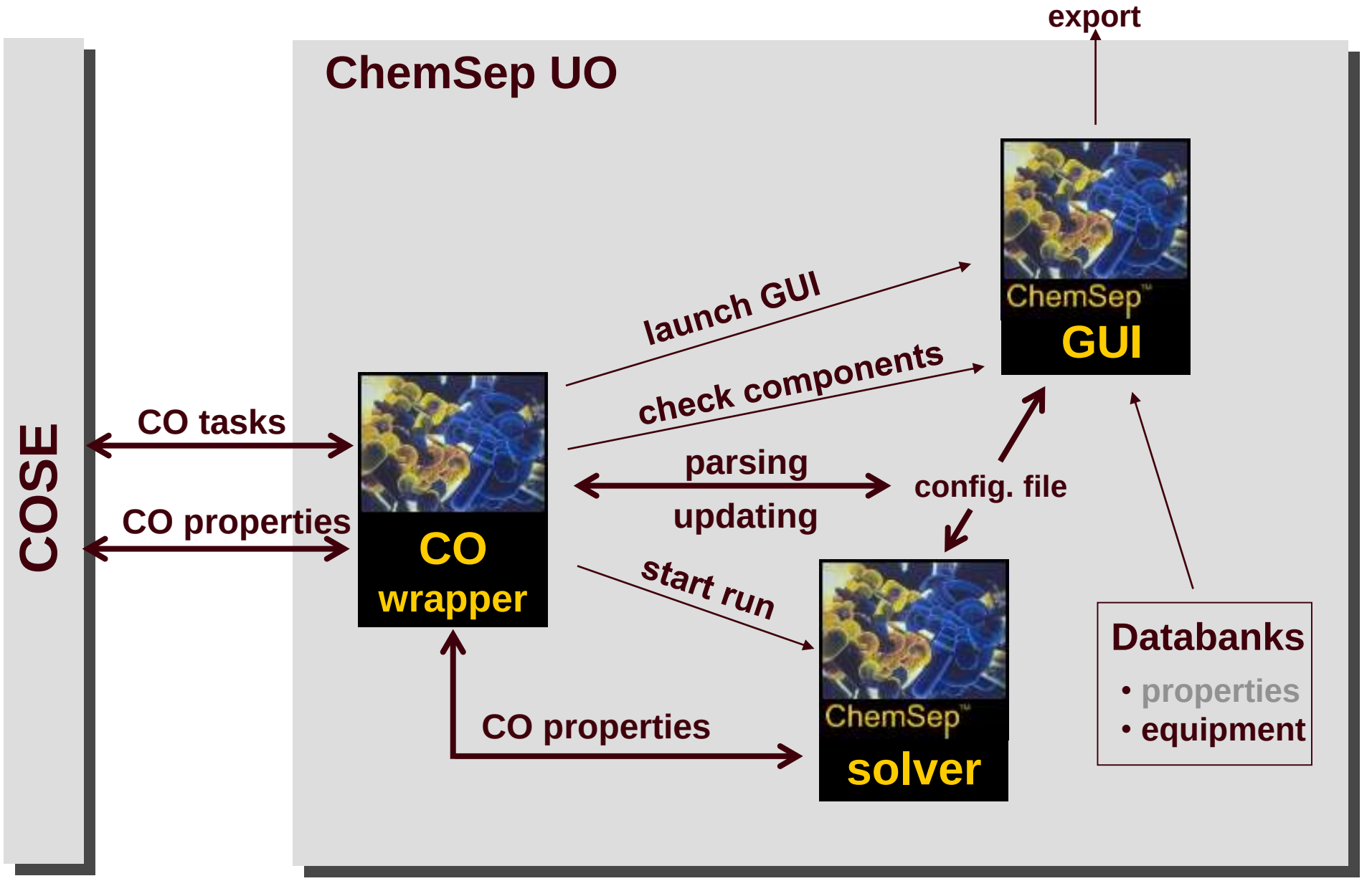
CO ChemSep Architecture: Phase I



CO ChemSep Architecture: Phase I



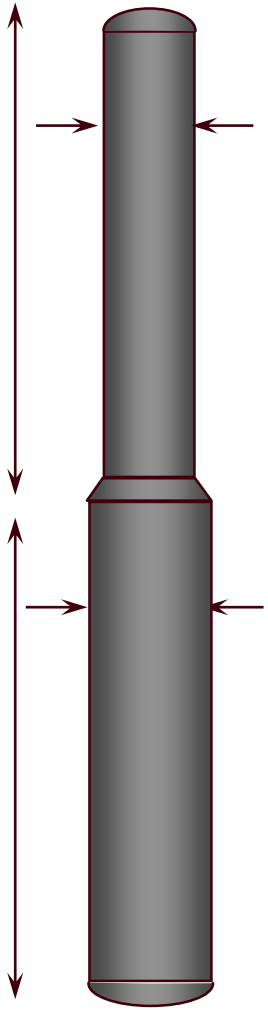
CO ChemSep Architecture: Phase II



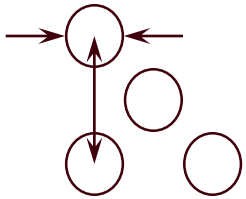
Two more concerns:

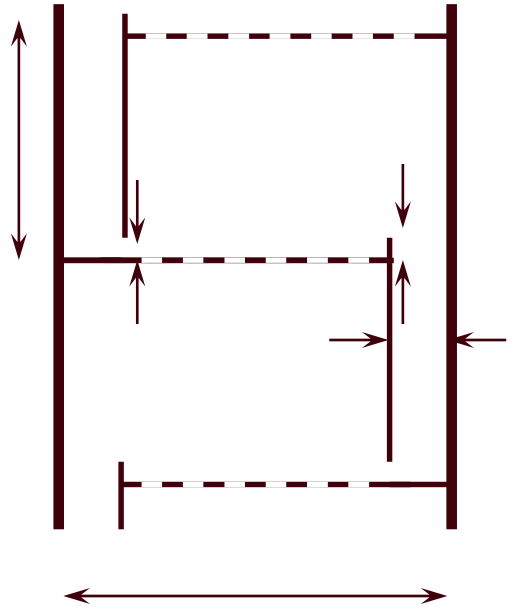
1. Equipment design
2. Physical Properties

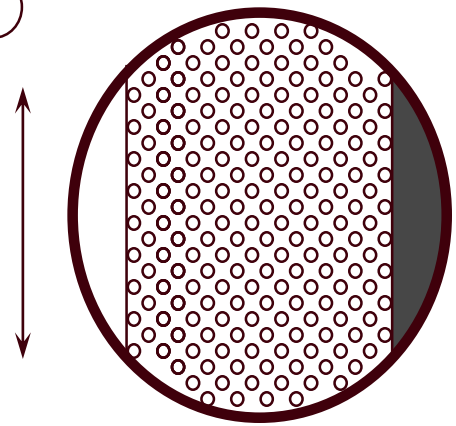
Equipment Design



- Bubble cap trays
- Sieve trays
- Valve trays
- Random packings
- Structured packings
- Rotating disc contactors
- and more

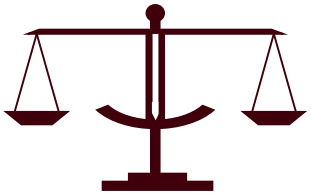






- **design mode**: computer
- **simulation**: own input!

Model requirements: Properties



Activity Coefficients
Vapor pressures
Fugacity coefficients

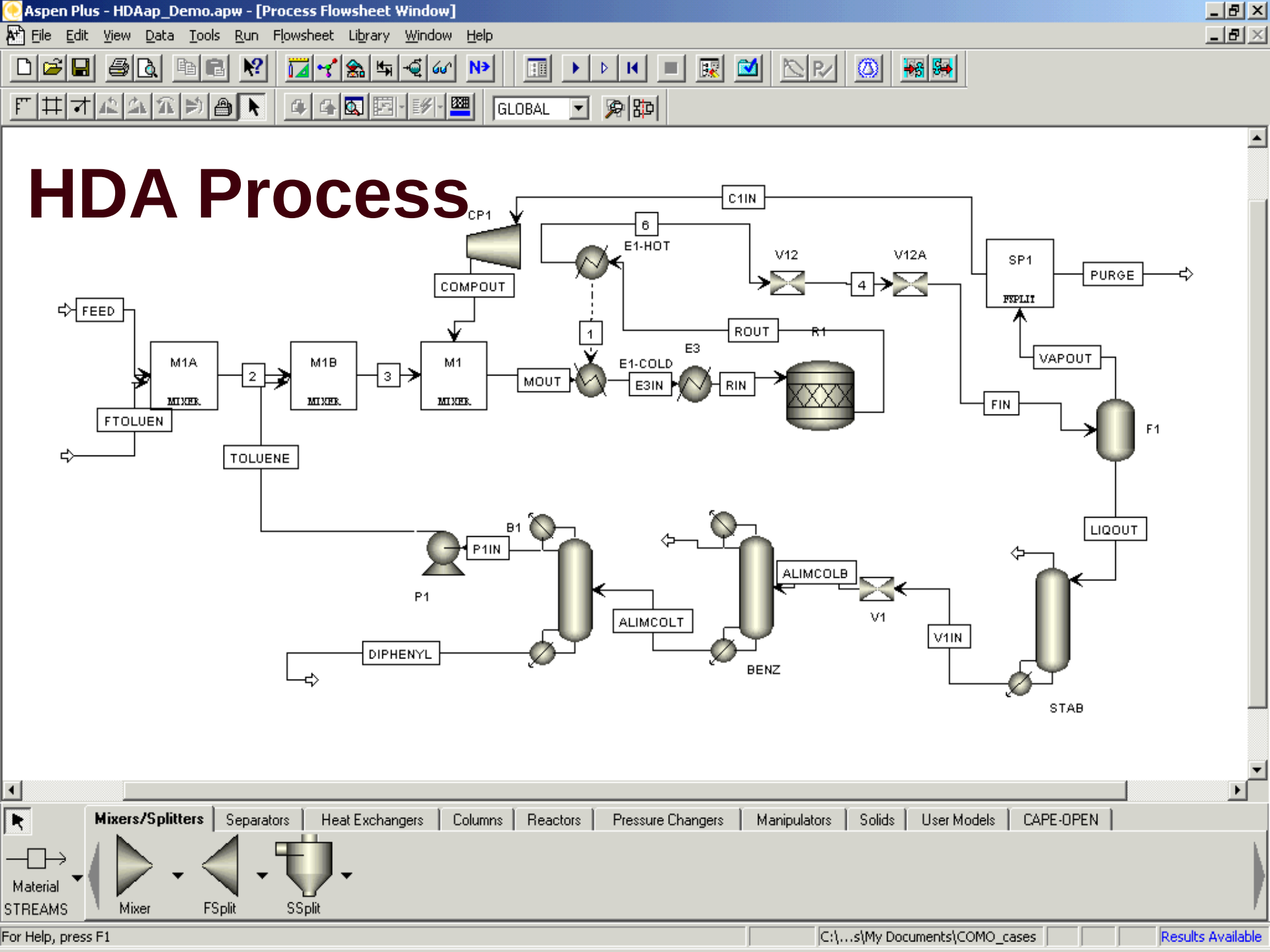
Heat capacities

K-values
Enthalpies

Densities
Viscosities
Surface tension
Thermal conductivities
Diffusion Coefficients

Interfacial areas
Mass transfer coefficients
Heat transfer coefficients

HDA Process



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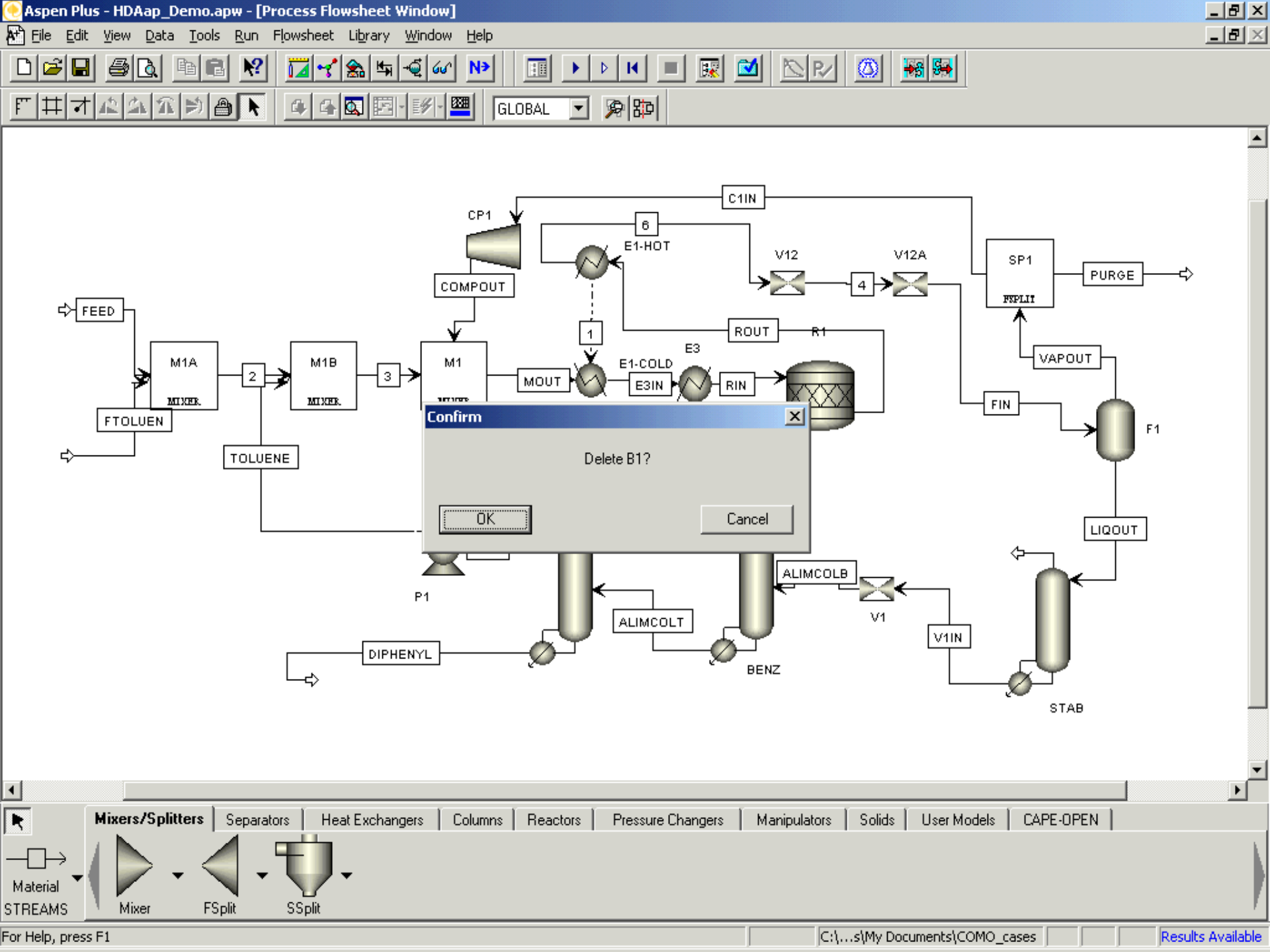
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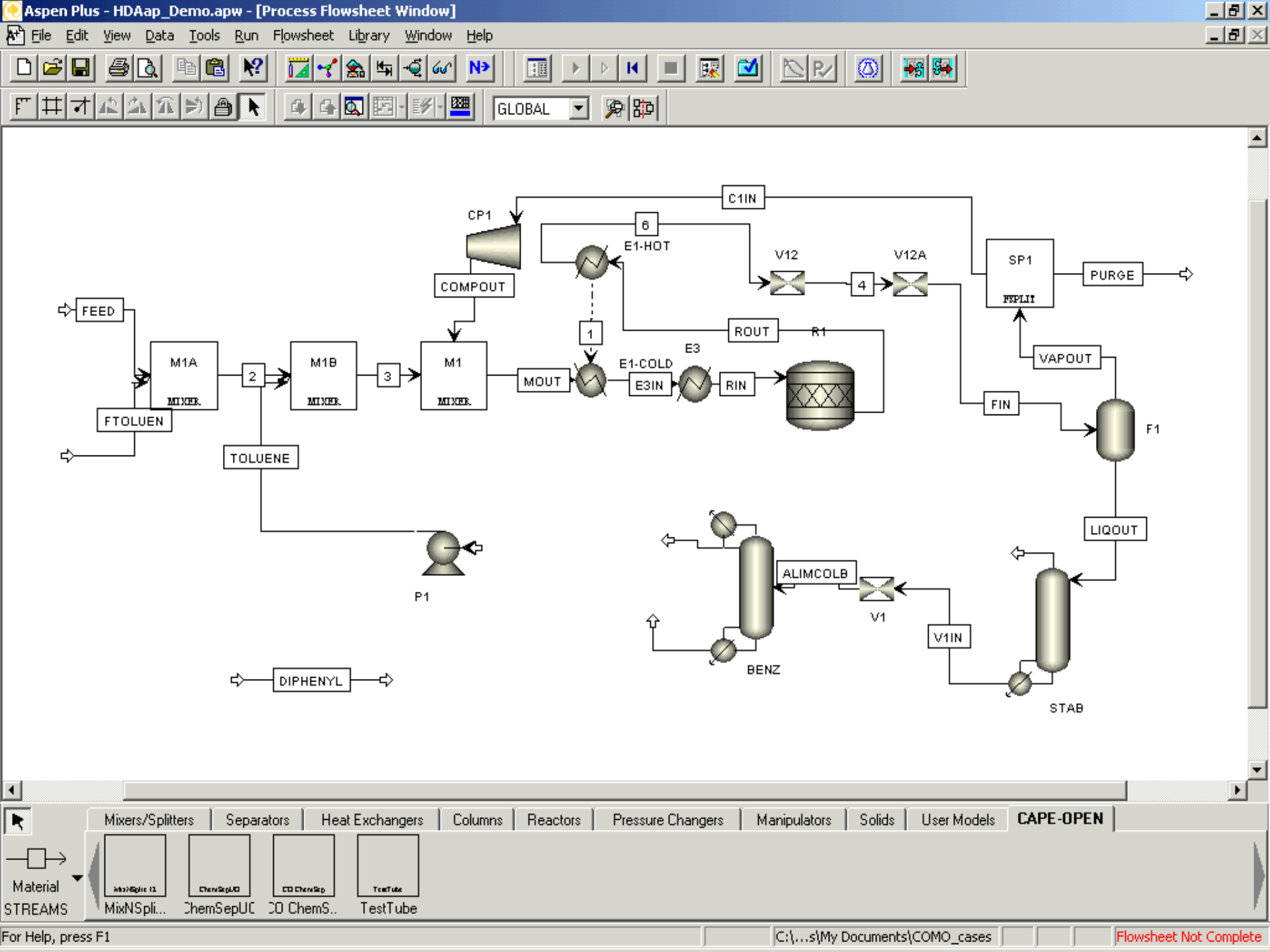
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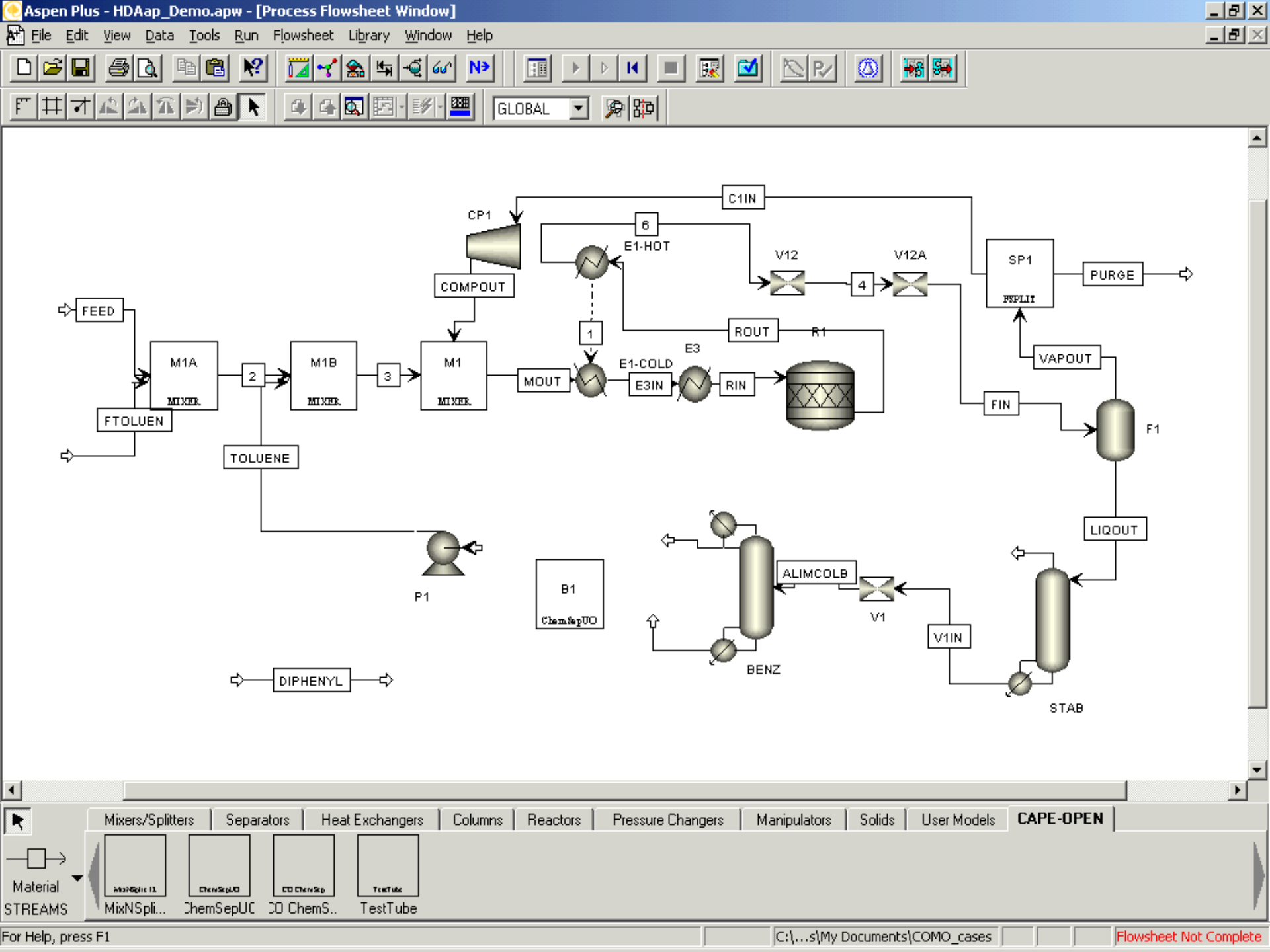
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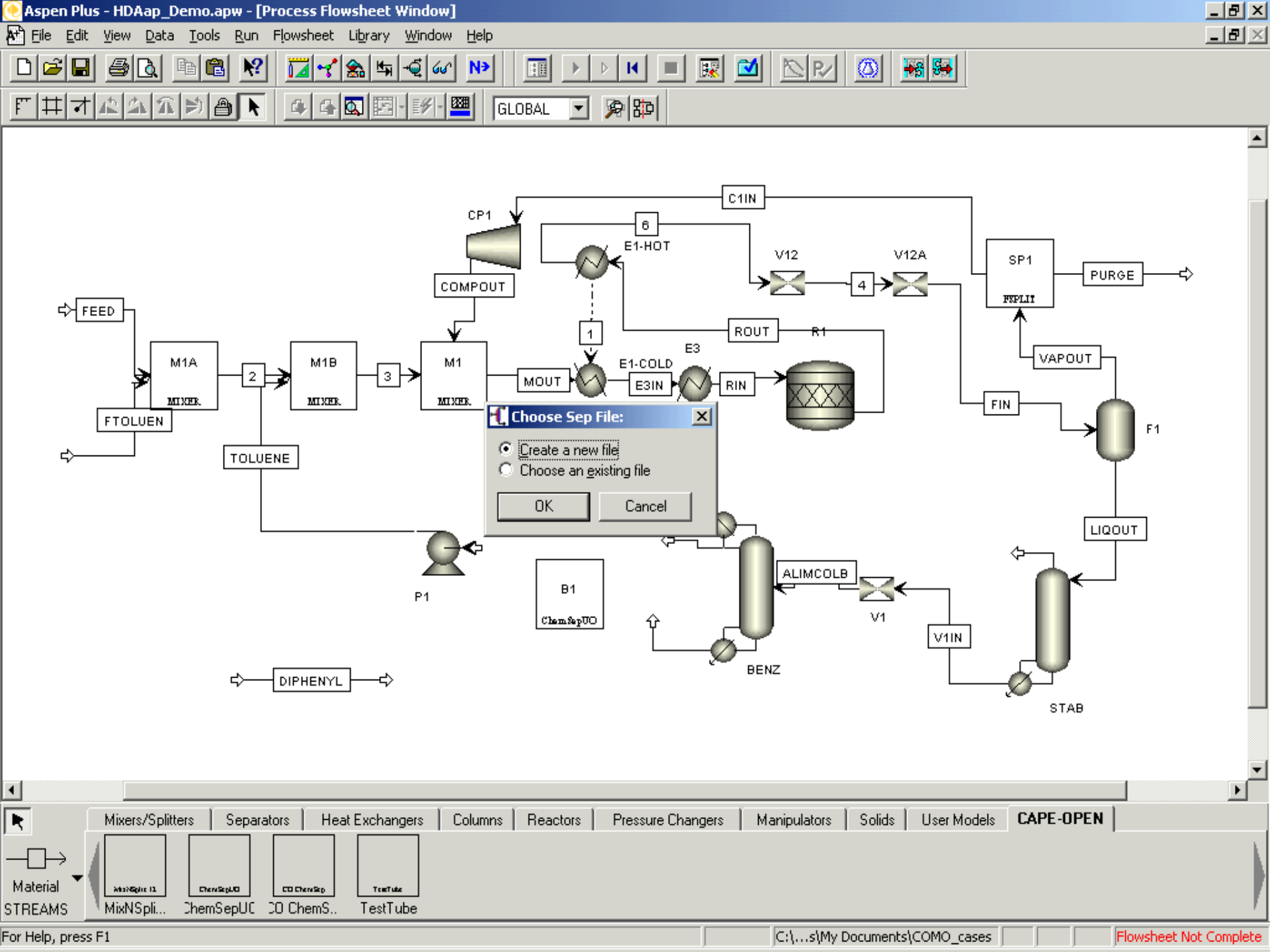
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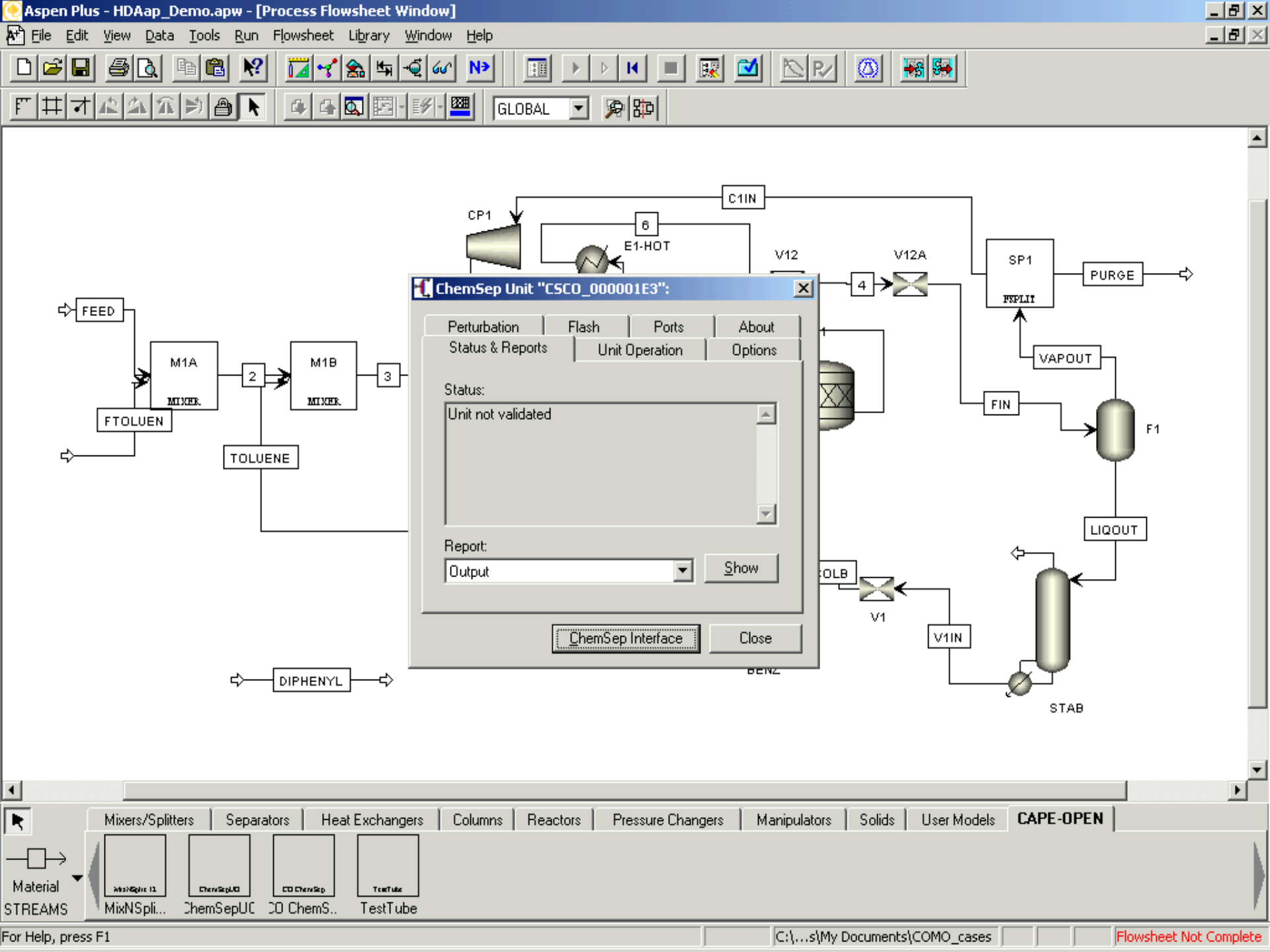
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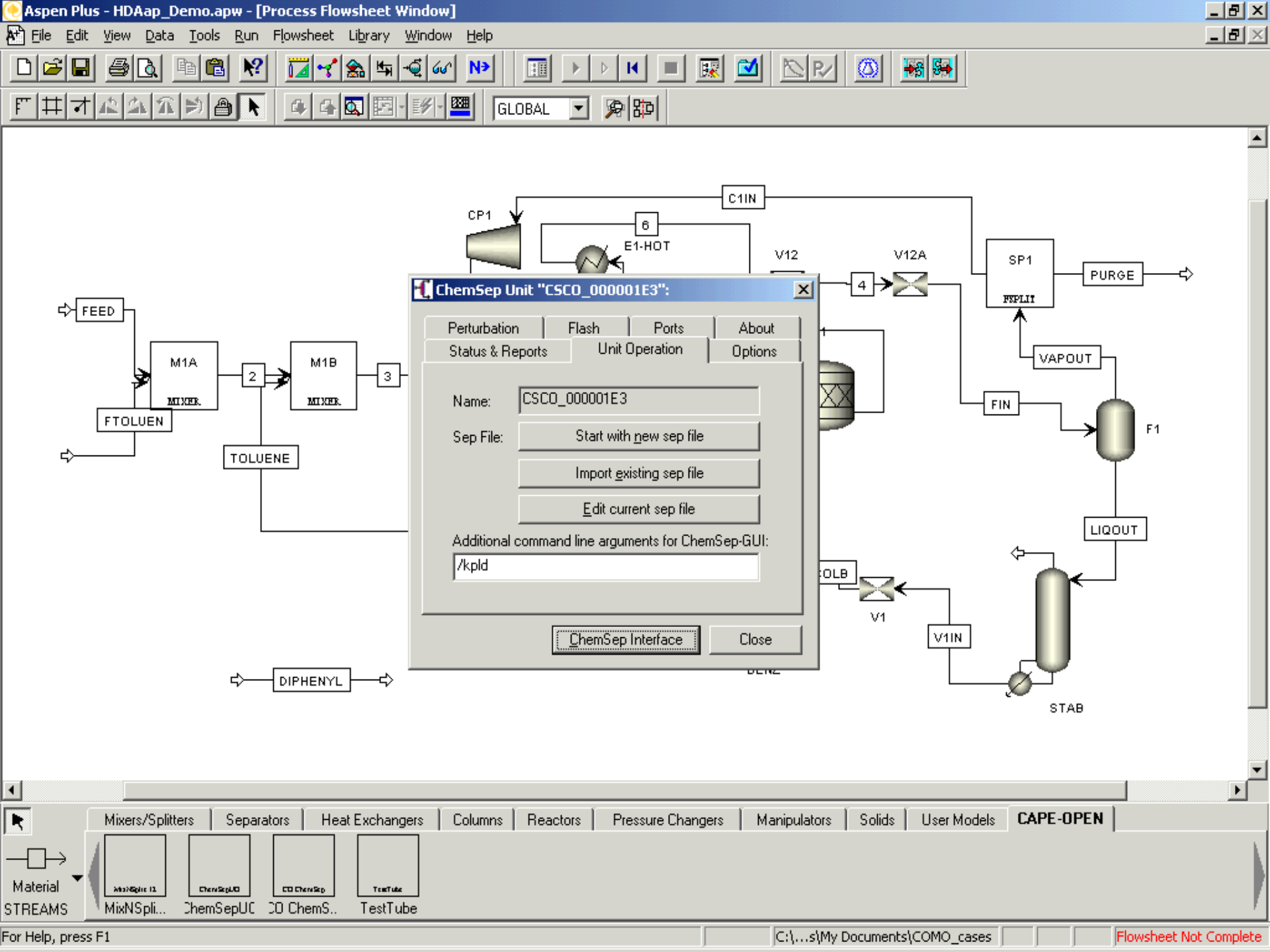
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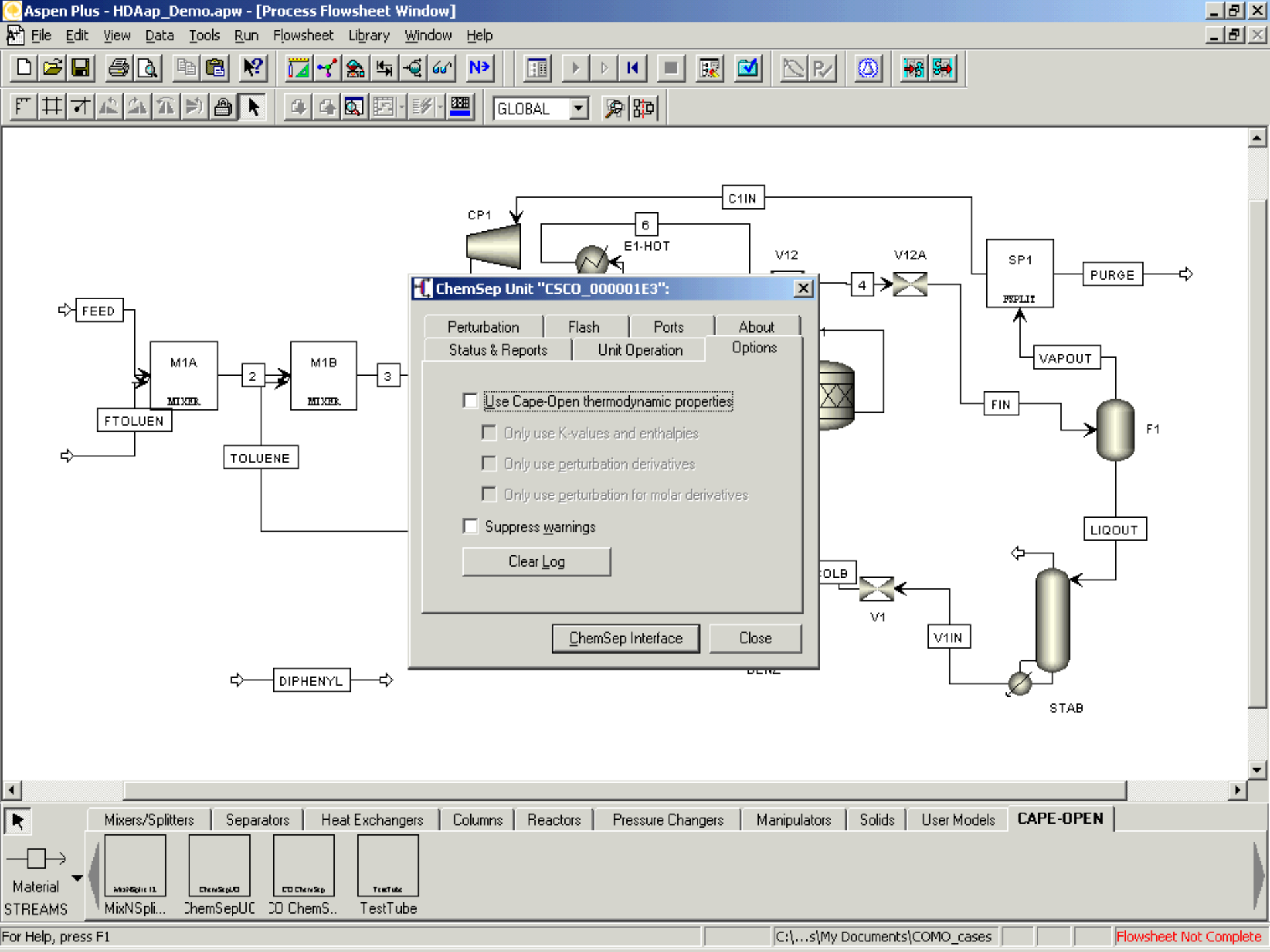
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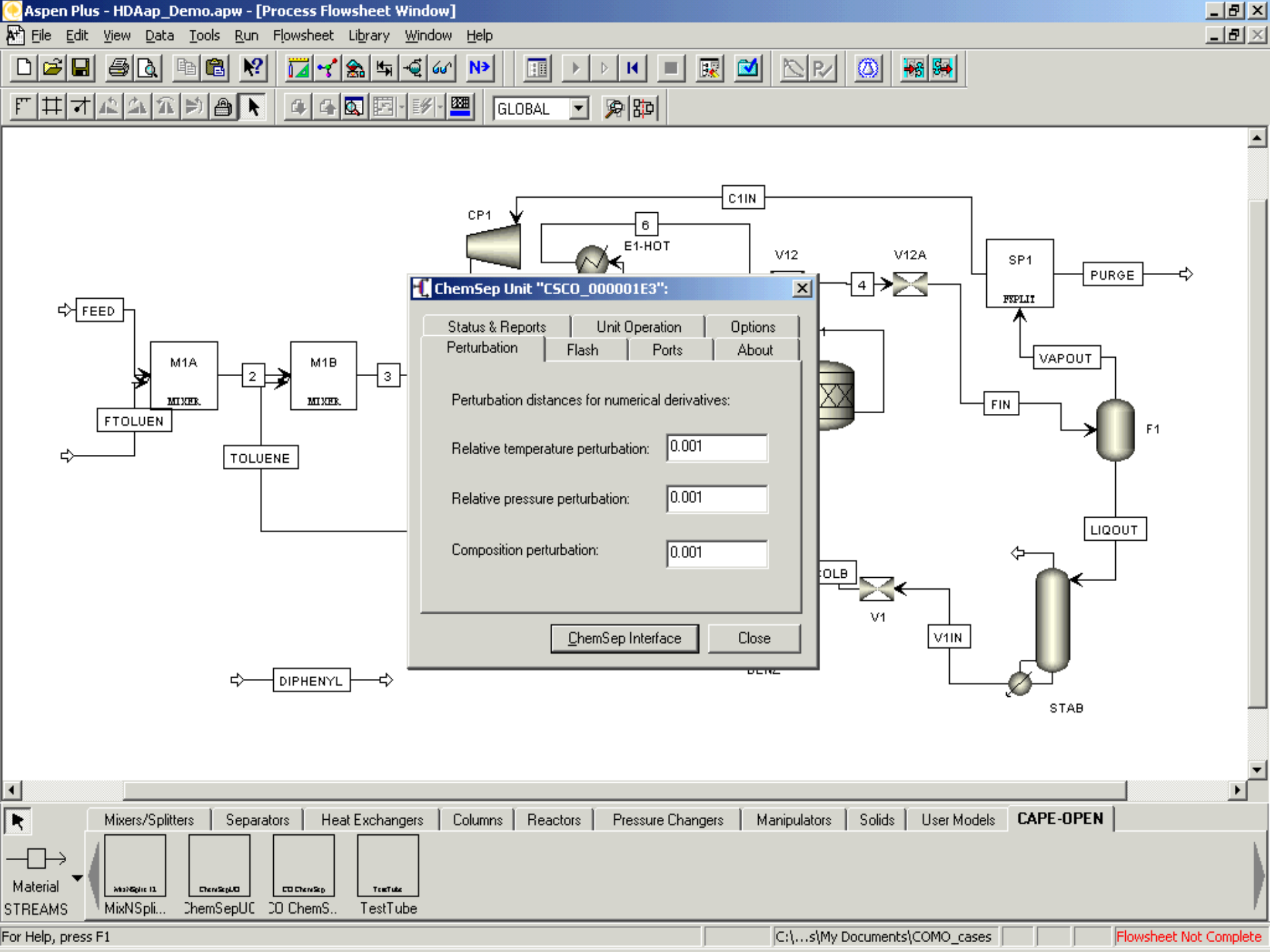
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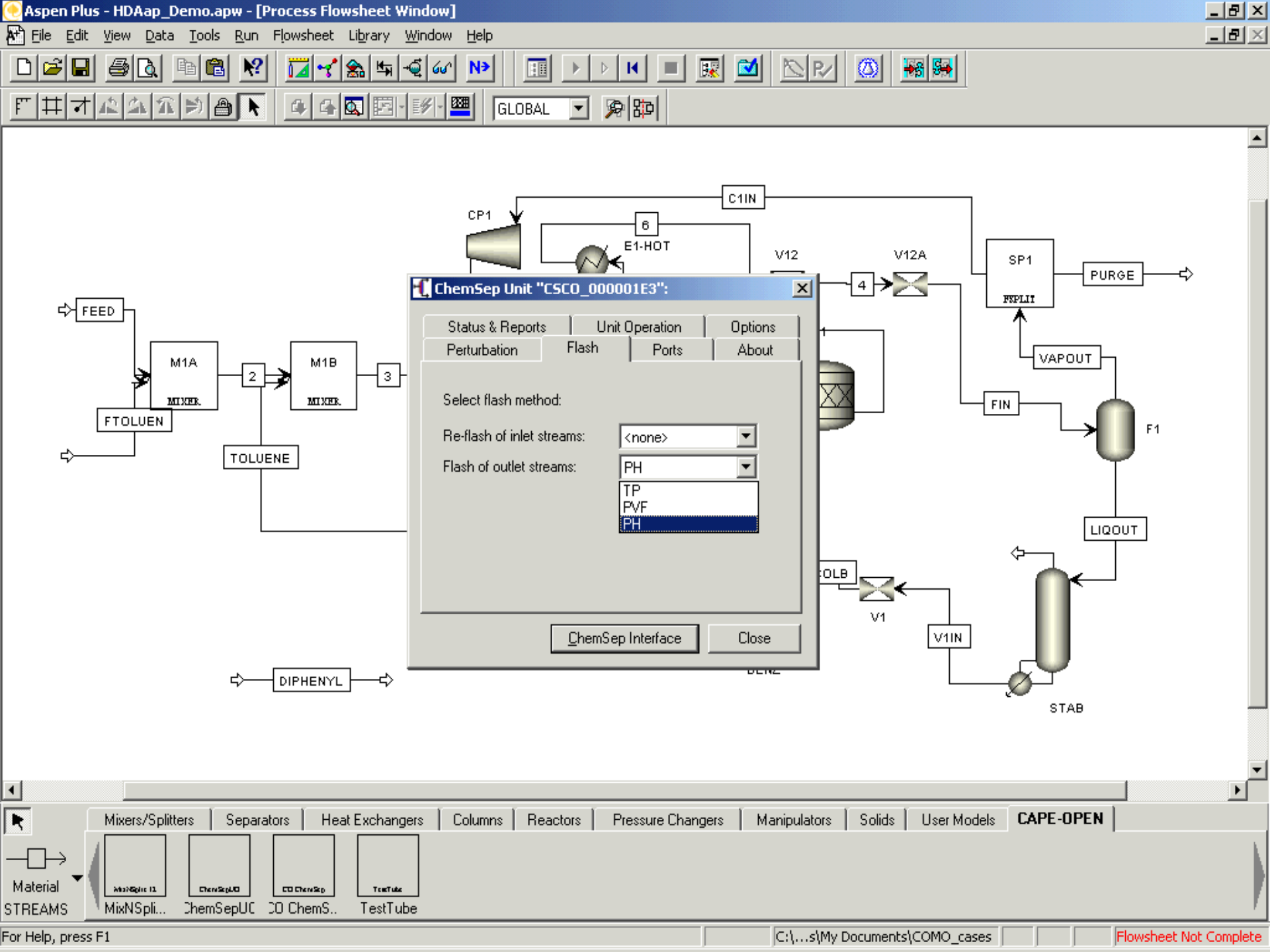
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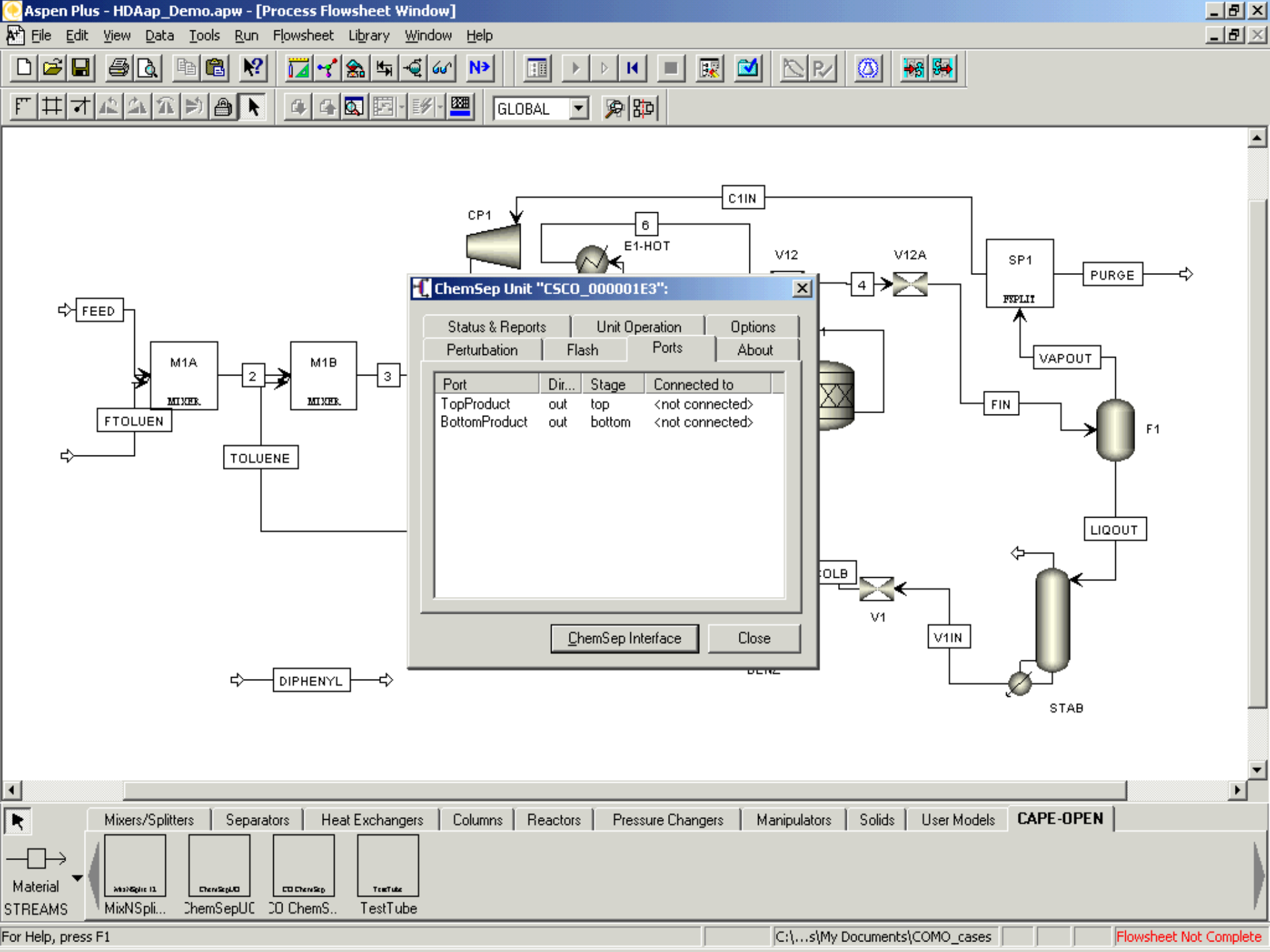
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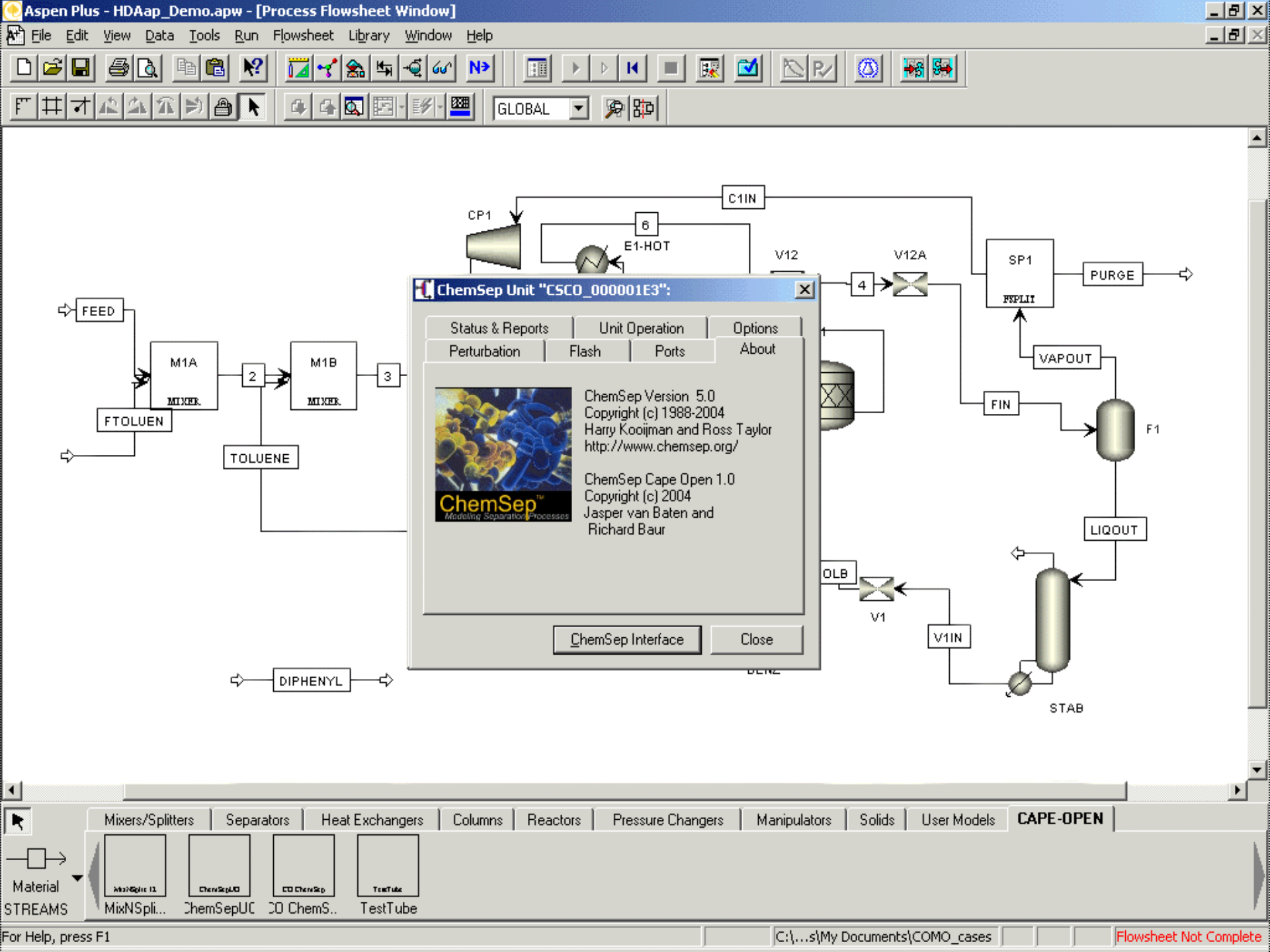
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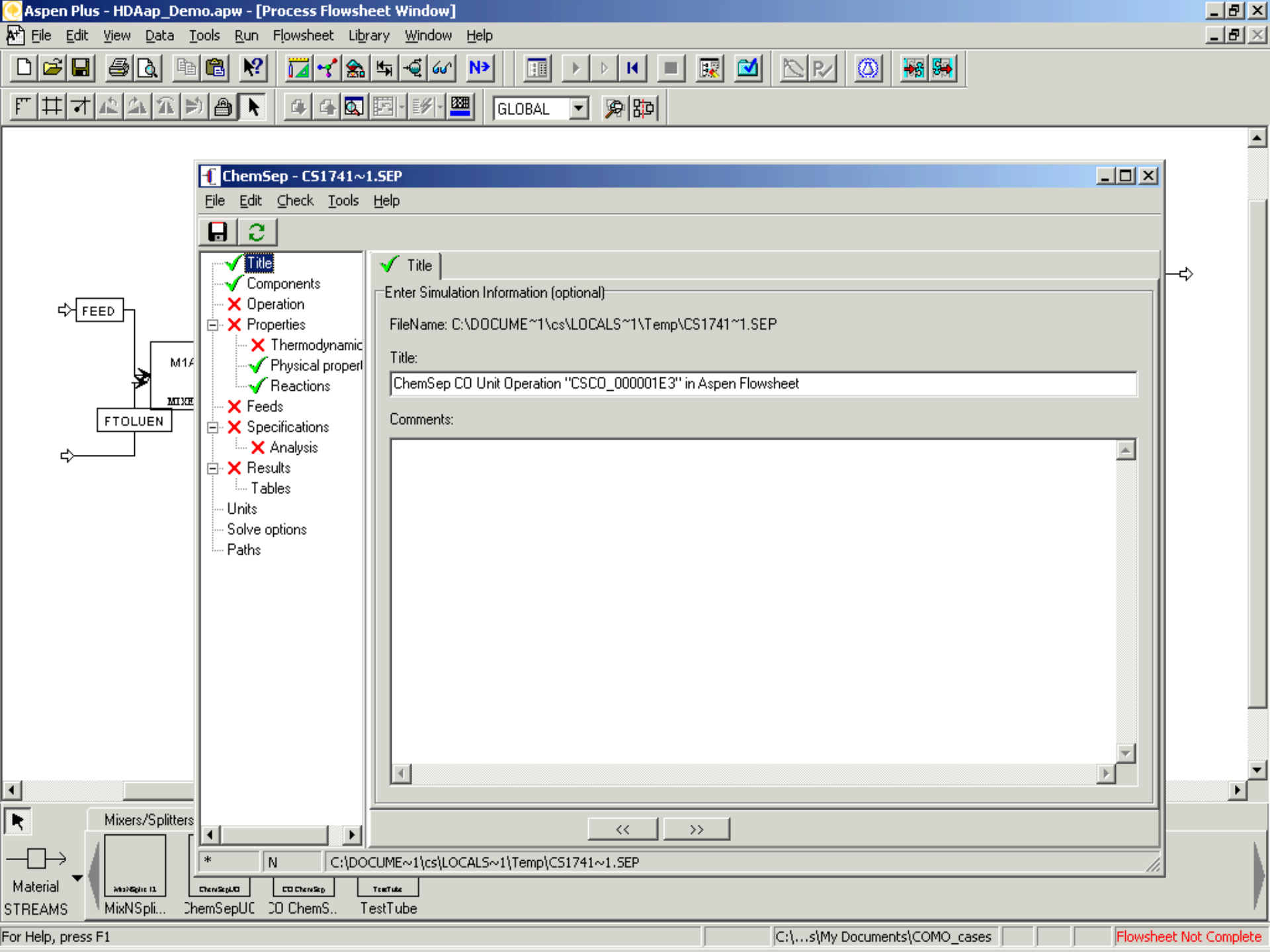
Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
ChemSep - CS1741~1.SEP
File Edit Check Tools Help
Title
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Enter Simulation Information (optional)
FileName: C:\DOCUME~1\cs\LOCALS~1\Temp\CS1741~1.SEP
Title:
ChemSep CO Unit Operation "CSCO_000001E3" in Aspen Flowsheet
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TestTube
For Help, press F1
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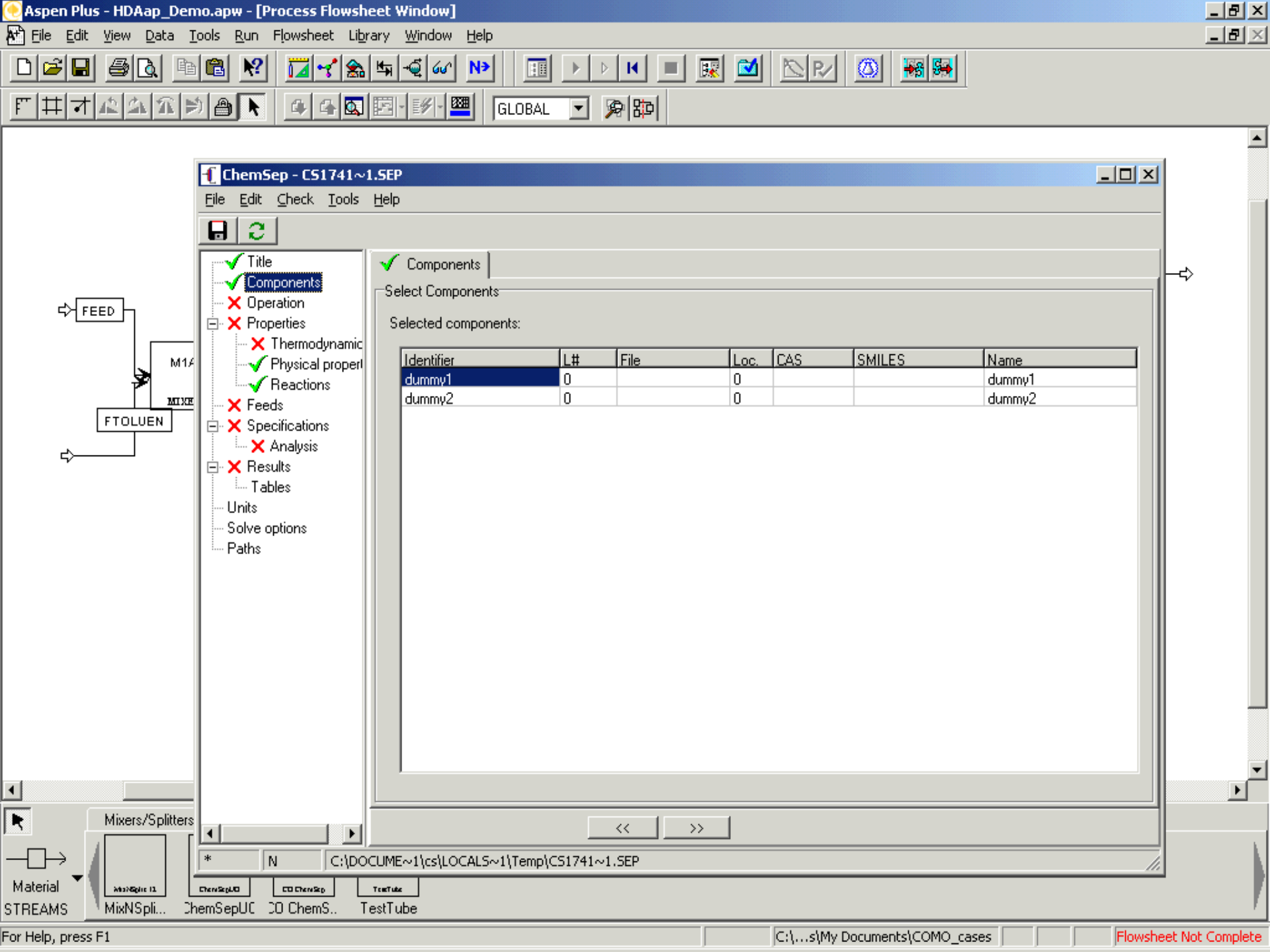
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Physical properl
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Feeds
Specifications
Analysis
Results
Tables
Units
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Paths
Components
Select Components
Selected components:
Identifier L# File Loc. CAS SMILES Name
dummy1 0 0 dummy1
dummy2 0 0 dummy2
<< >>
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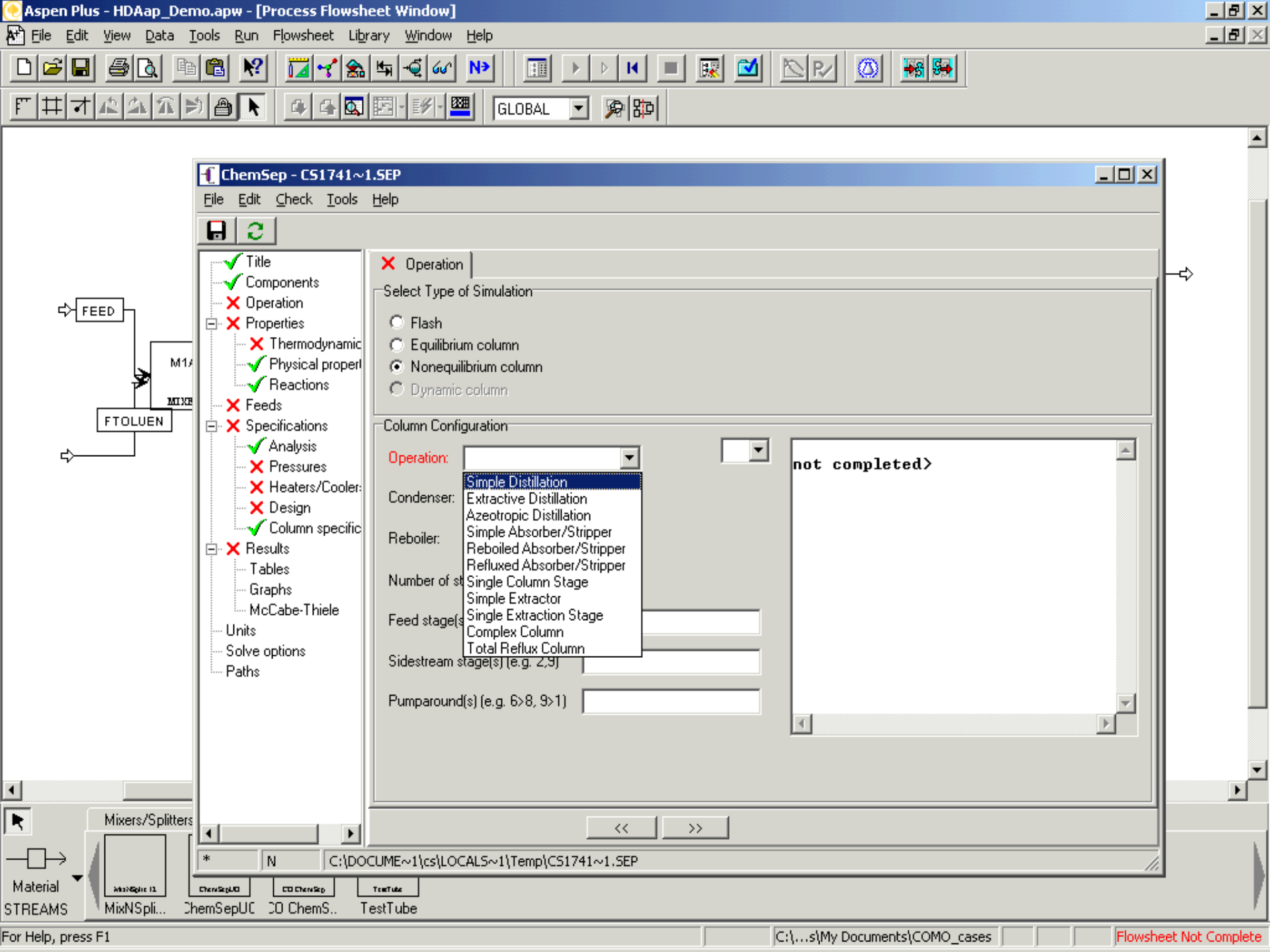
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Heaters/Cooler:
Design
Column specific
Results
Tables
Graphs
McCabe-Thiele
Units
Solve options
Paths
Operation
Select Type of Simulation
Flash
Equilibrium column
Nonequilibrium column
Dynamic column
Column Configuration
Operation:
Condenser:
Reboiler:
Number of st
Feed stage(s
Sidestream stage(s) (e.g. 2;9)
Pumparound(s) (e.g. 6>8, 9>1)
Simple Distillation
Extractive Distillation
Azeotropic Distillation
Simple Absorber/Stripper
Reboiled Absorber/Stripper
Refluxed Absorber/Stripper
Single Column Stage
Simple Extractor
Single Extraction Stage
Complex Column
Total Reflux Column
not completed>
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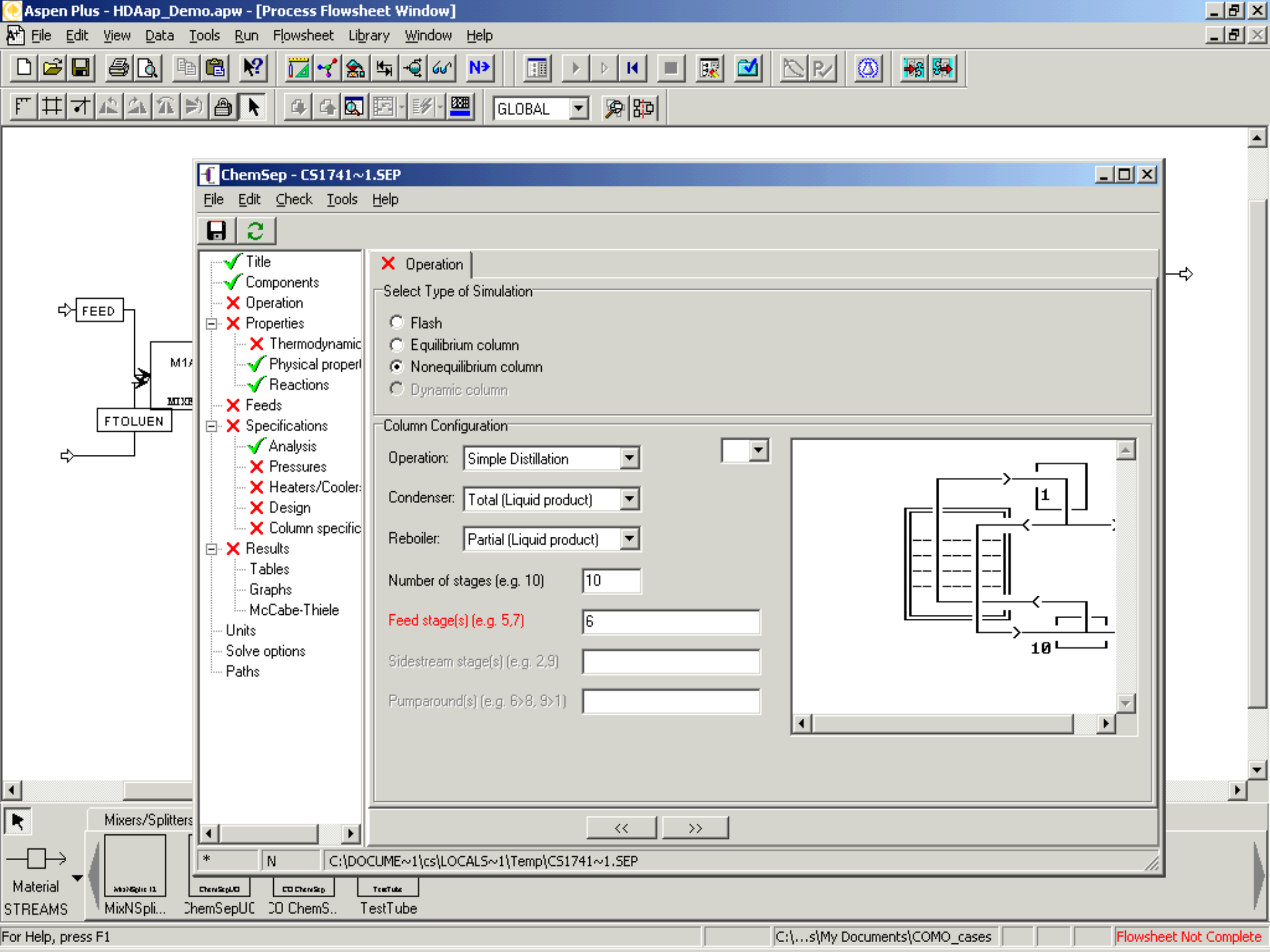
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Heaters/Cooler:
Design
Column specific
Results
Tables
Graphs
McCabe-Thiele
Units
Solve options
Paths
Operation
Select Type of Simulation
Flash
Equilibrium column
Nonequilibrium column
Dynamic column
Column Configuration
Operation: Simple Distillation
Condenser: Total (Liquid product)
Reboiler: Partial (Liquid product)
Number of stages (e.g. 10) 10
Feed stage(s) (e.g. 5,7) 6
Sidestream stage(s) (e.g. 2,9)
Pumparound(s) (e.g. 6>8, 9>1)
1
10
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TestTube
For Help, press F1
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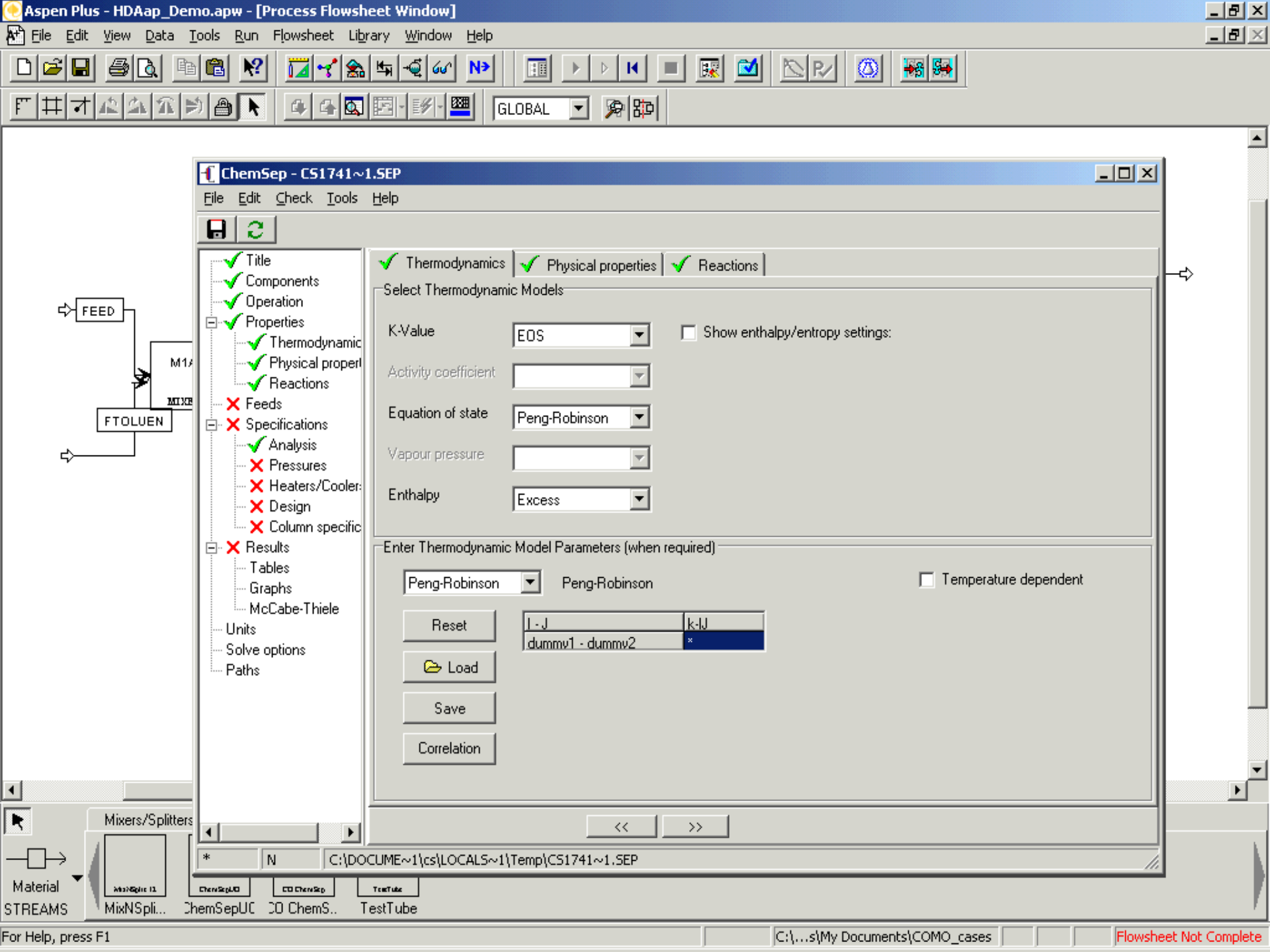
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Paths
Thermodynamics
Physical properties
Reactions
Select Thermodynamic Models
K-Value
EOS
Show enthalpy/entropy settings:
Activity coefficient
Equation of state
Peng-Robinson
Vapour pressure
Enthalpy
Excess
Enter Thermodynamic Model Parameters (when required)
Peng-Robinson
Peng-Robinson
Temperature dependent
Reset
Load
Save
Correlation
i - j
k-ij
dummy1 - dummy2
<<
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TestTube
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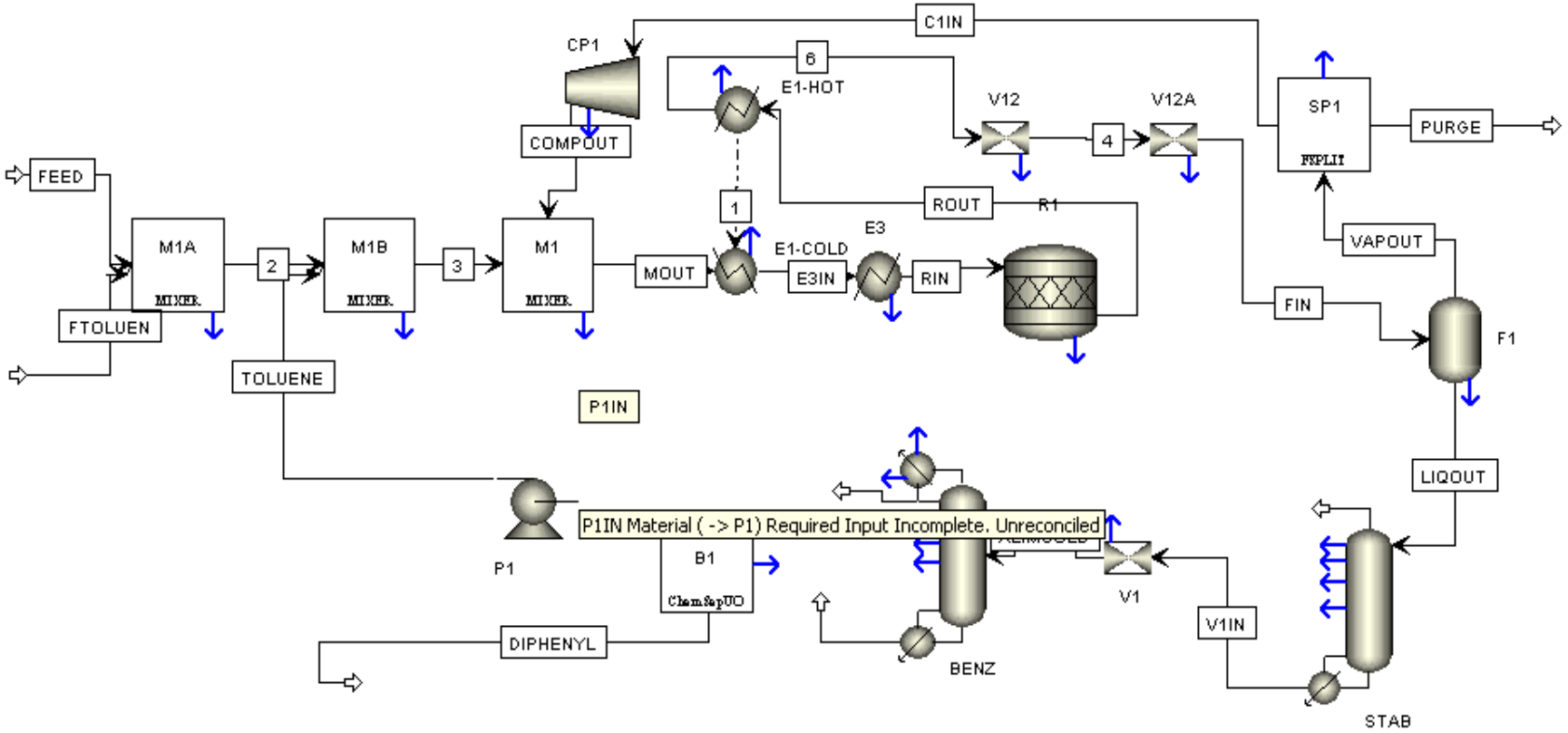
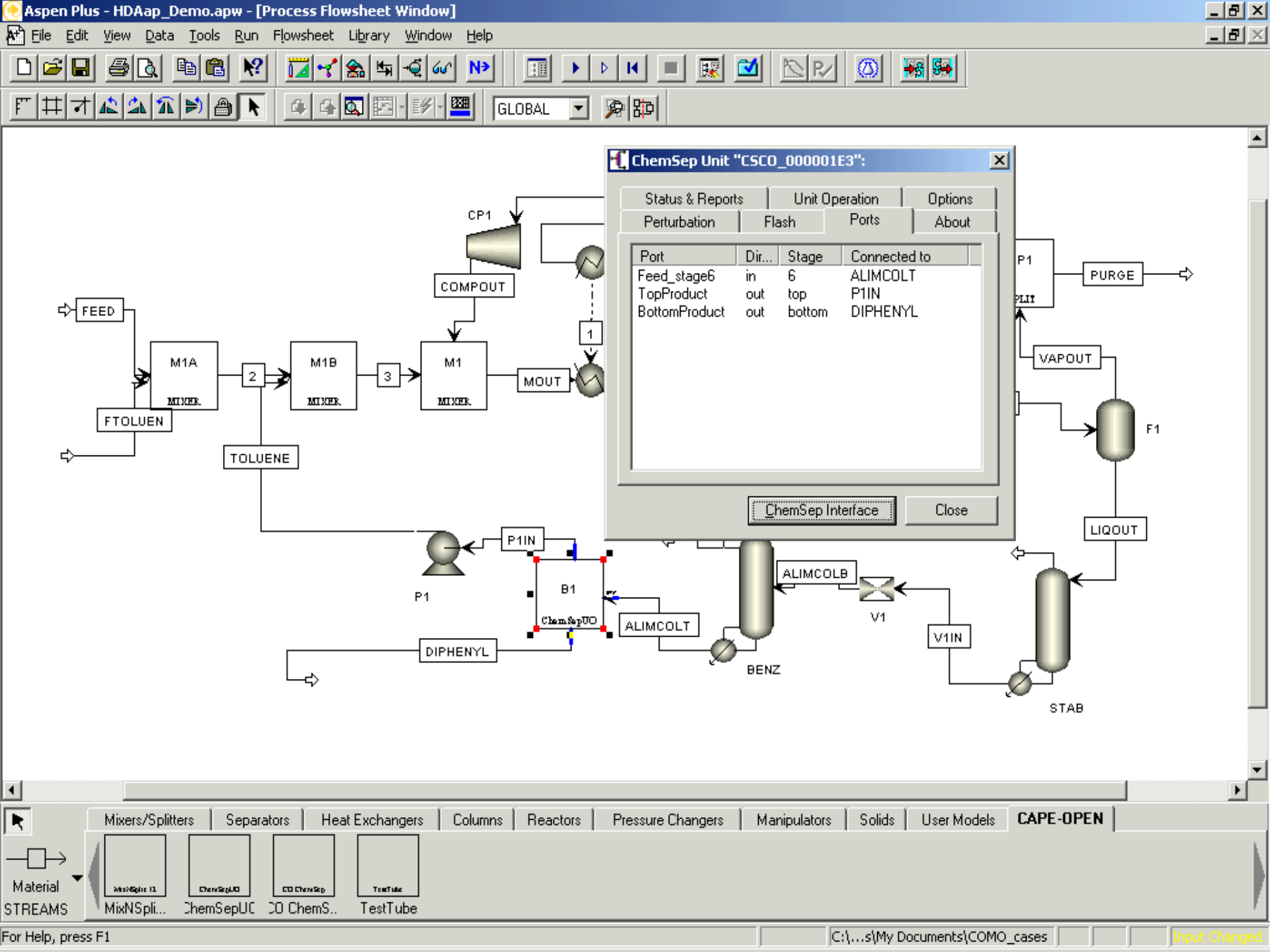


Mixers/Splitters | Separators | Heat Exchangers | Columns | Reactors | Pressure Changers | Manipulators | Solids | User Models | CAPE-OPEN

Material STREAMS

MixNSpli... ChemSepUC CO ChemS.. TestTube

For Help, press F1 | C:\...s\My Documents\COMO_cases | Required Input Incomplete


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
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ChemSep Unit "CSCO_000001E3":
Status & Reports
Unit Operation
Options
Perturbation
Flash
Ports
About
Port Dir... Stage Connected to
Feed_stage6 in 6 ALIMCOLT
TopProduct out top P1IN
BottomProduct out bottom DIPHENYL
ChemSep Interface
Close
CP1
COMPOUT
FEED
M1A
MIXER
2
M1B
MIXER
3
M1
MIXER
MOUT
1
FTOLUEN
TOLUENE
P1
P1IN
B1
ChemSepUO
ALIMCOLT
DIPHENYL
ALIMCOLB
V1
V1IN
BENZ
STAB
P1
PURGE
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Mixers/Splitters
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Heat Exchangers
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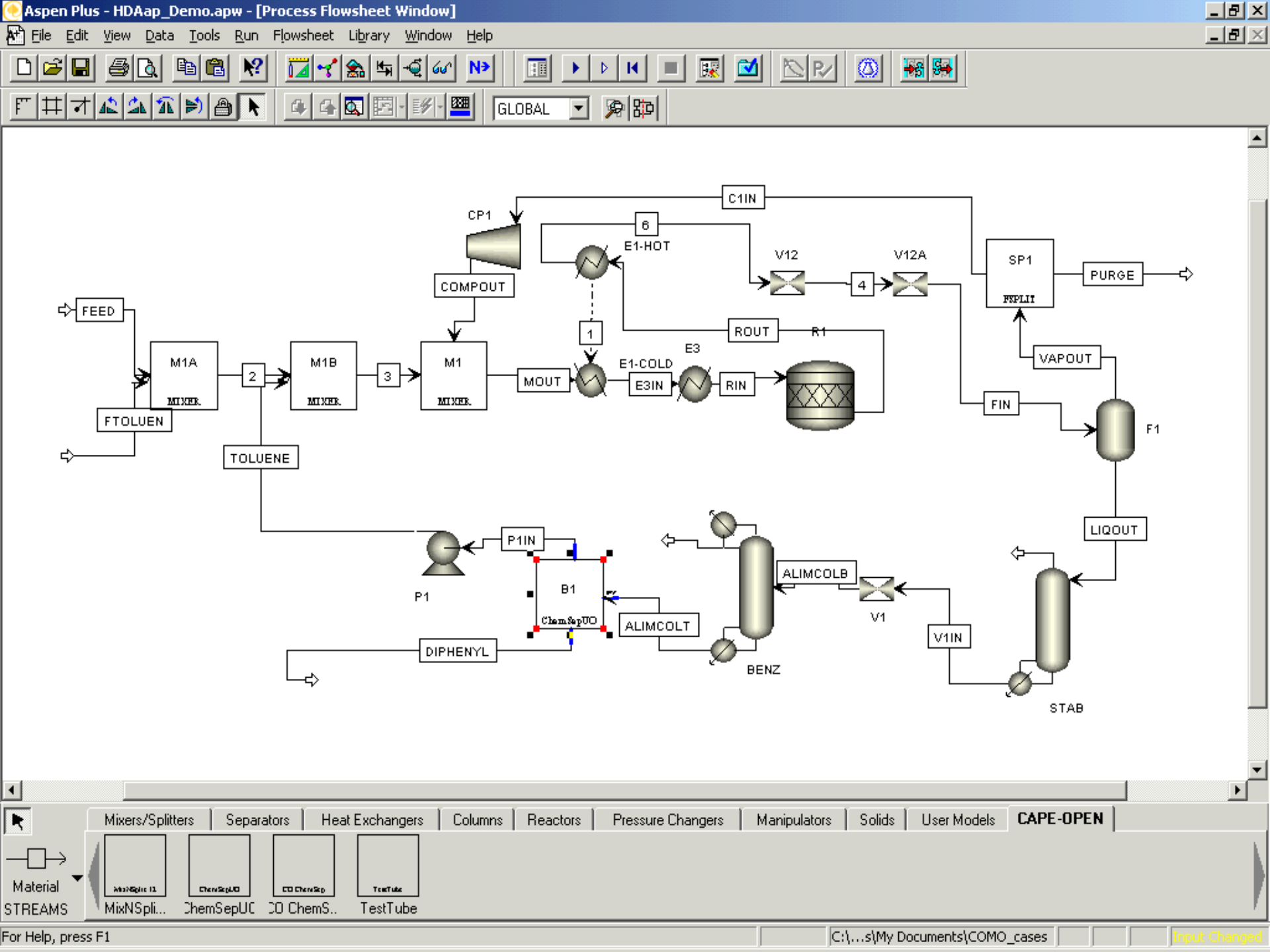
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6
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COMPOUT
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E1-COLD
VAPOUT
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M1
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E3IN
RIN
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TOLUENE
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LIQOUT
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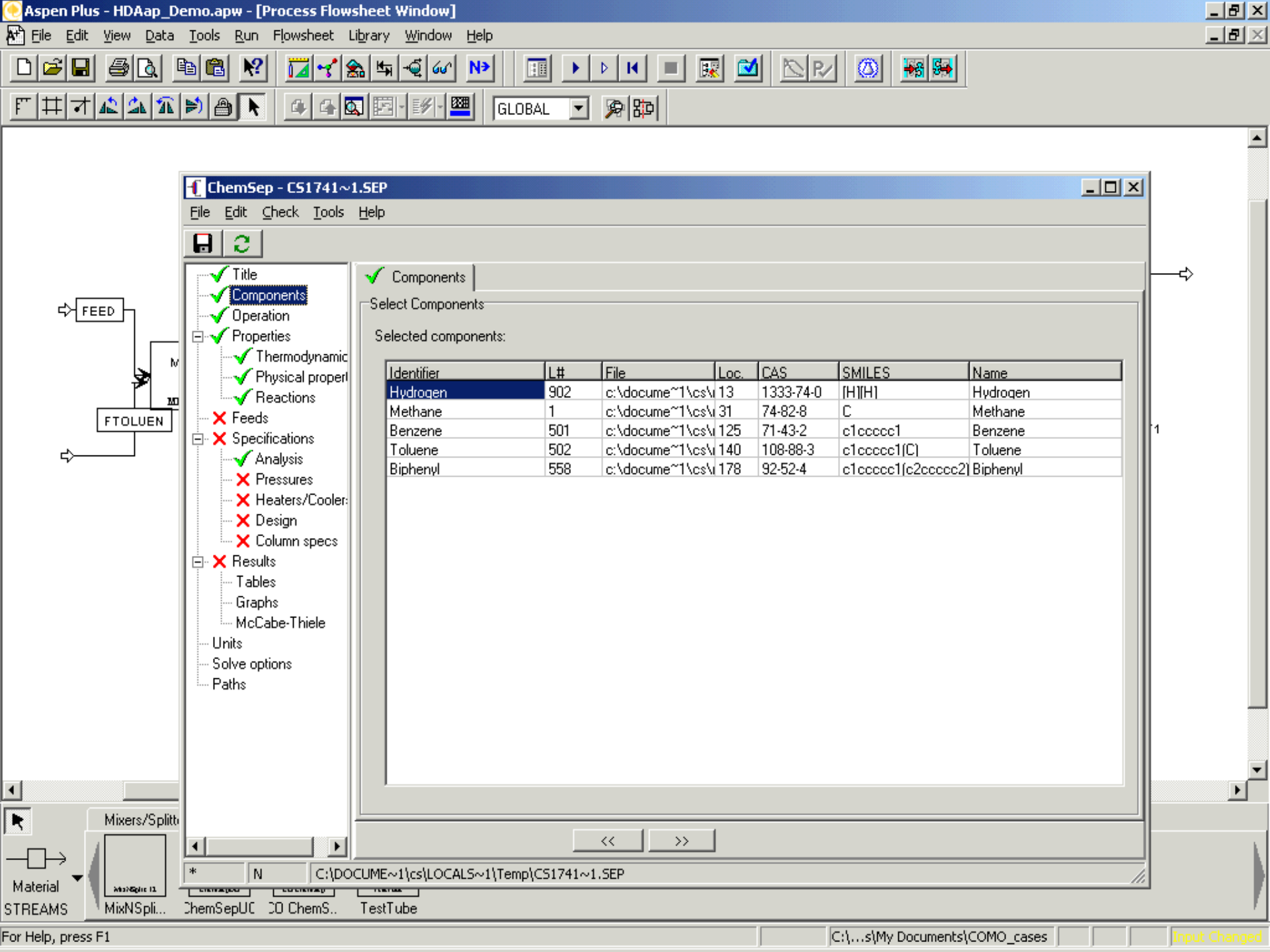
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Graphs
McCabe-Thiele
Units
Solve options
Paths
Components
Select Components
Selected components:
Identifier L# File Loc. CAS SMILES Name
Hydrogen 902 c:\docume~1\cs\l 13 1333-74-0 [H][H] Hydrogen
Methane 1 c:\docume~1\cs\l 31 74-82-8 C Methane
Benzene 501 c:\docume~1\cs\l 125 71-43-2 c1ccccc1 Benzene
Toluene 502 c:\docume~1\cs\l 140 108-88-3 c1ccccc1(C) Toluene
Biphenyl 558 c:\docume~1\cs\l 178 92-52-4 c1ccccc1(c2ccccc2) Biphenyl
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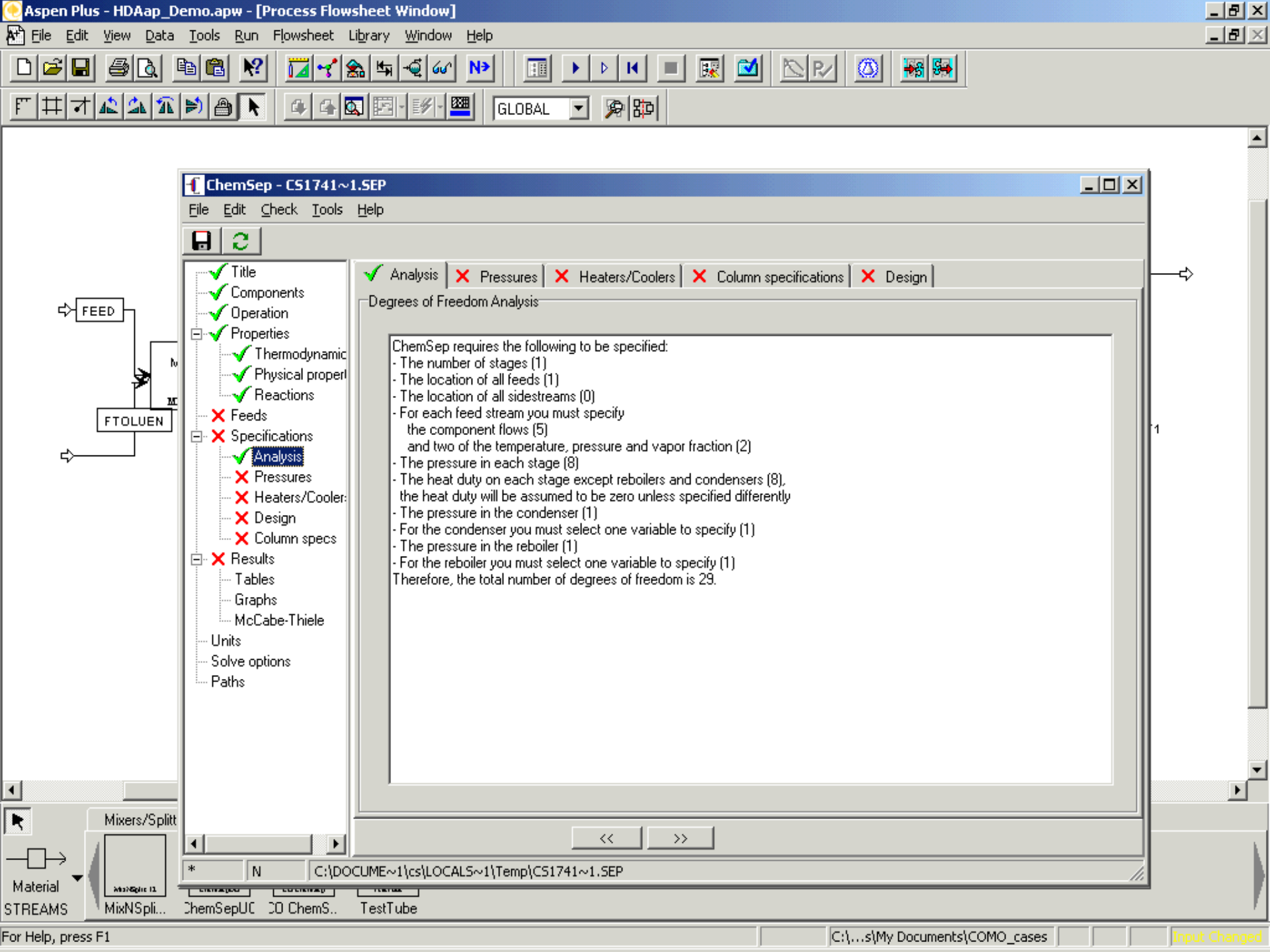
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Degrees of Freedom Analysis
ChemSep requires the following to be specified:
- The number of stages (1)
- The location of all feeds (1)
- The location of all sidestreams (0)
- For each feed stream you must specify
the component flows (5)
and two of the temperature, pressure and vapor fraction (2)
- The pressure in each stage (8)
- The heat duty on each stage except reboilers and condensers (8),
the heat duty will be assumed to be zero unless specified differently
- The pressure in the condenser (1)
- For the condenser you must select one variable to specify (1)
- The pressure in the reboiler (1)
- For the reboiler you must select one variable to specify (1)
Therefore, the total number of degrees of freedom is 29.
<< >>
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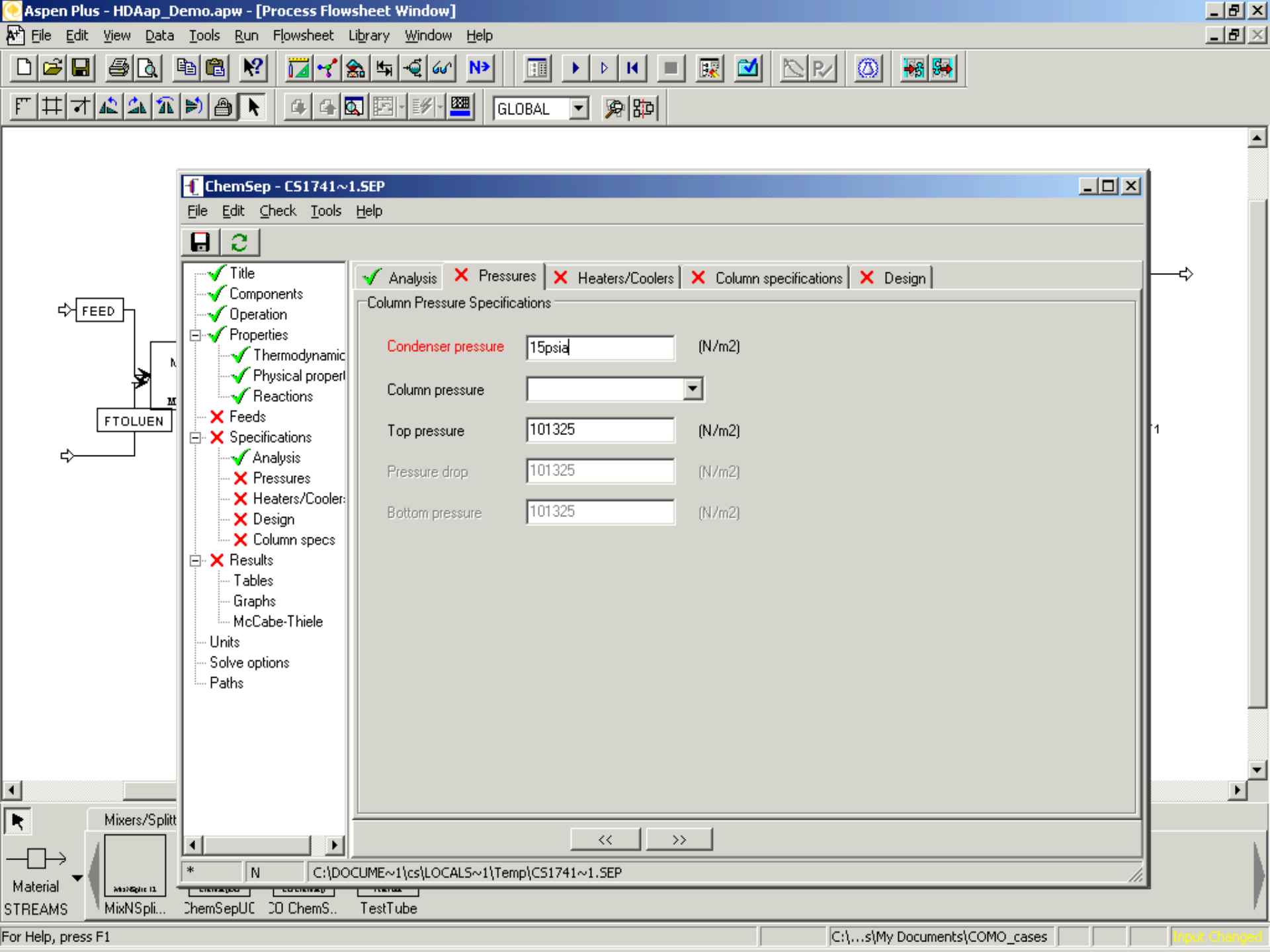
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Graphs
McCabe-Thiele
Units
Solve options
Paths
Analysis
Pressures
Heaters/Coolers
Column specifications
Design
Column Pressure Specifications
Condenser pressure
15psia
(N/m2)
Column pressure
Top pressure
101325
(N/m2)
Pressure drop
101325
(N/m2)
Bottom pressure
101325
(N/m2)
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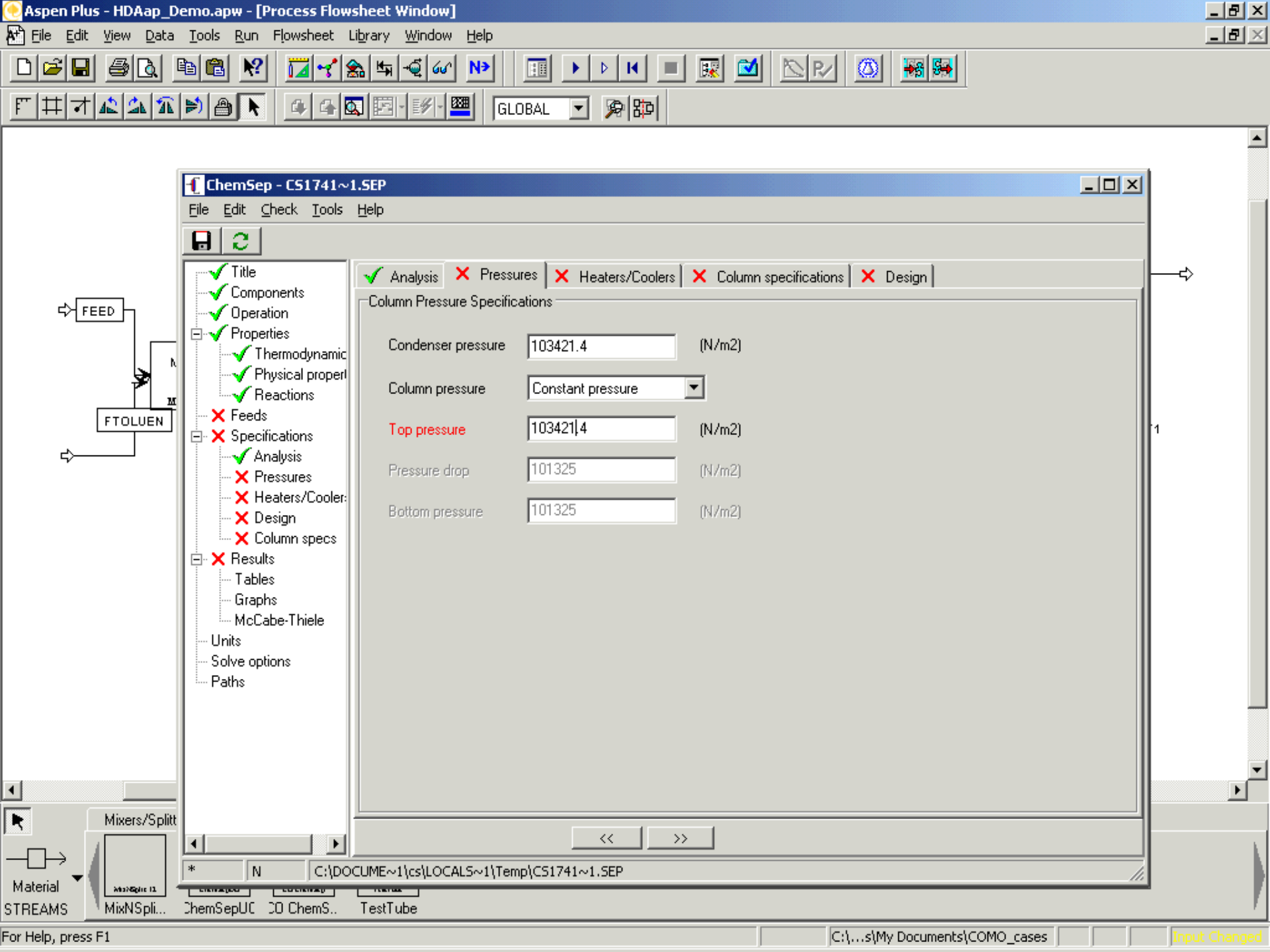
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Pressures
Heaters/Coolers
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Design
Column Pressure Specifications
Condenser pressure
103421.4
(N/m2)
Column pressure
Constant pressure
Top pressure
103421.4
(N/m2)
Pressure drop
101325
(N/m2)
Bottom pressure
101325
(N/m2)
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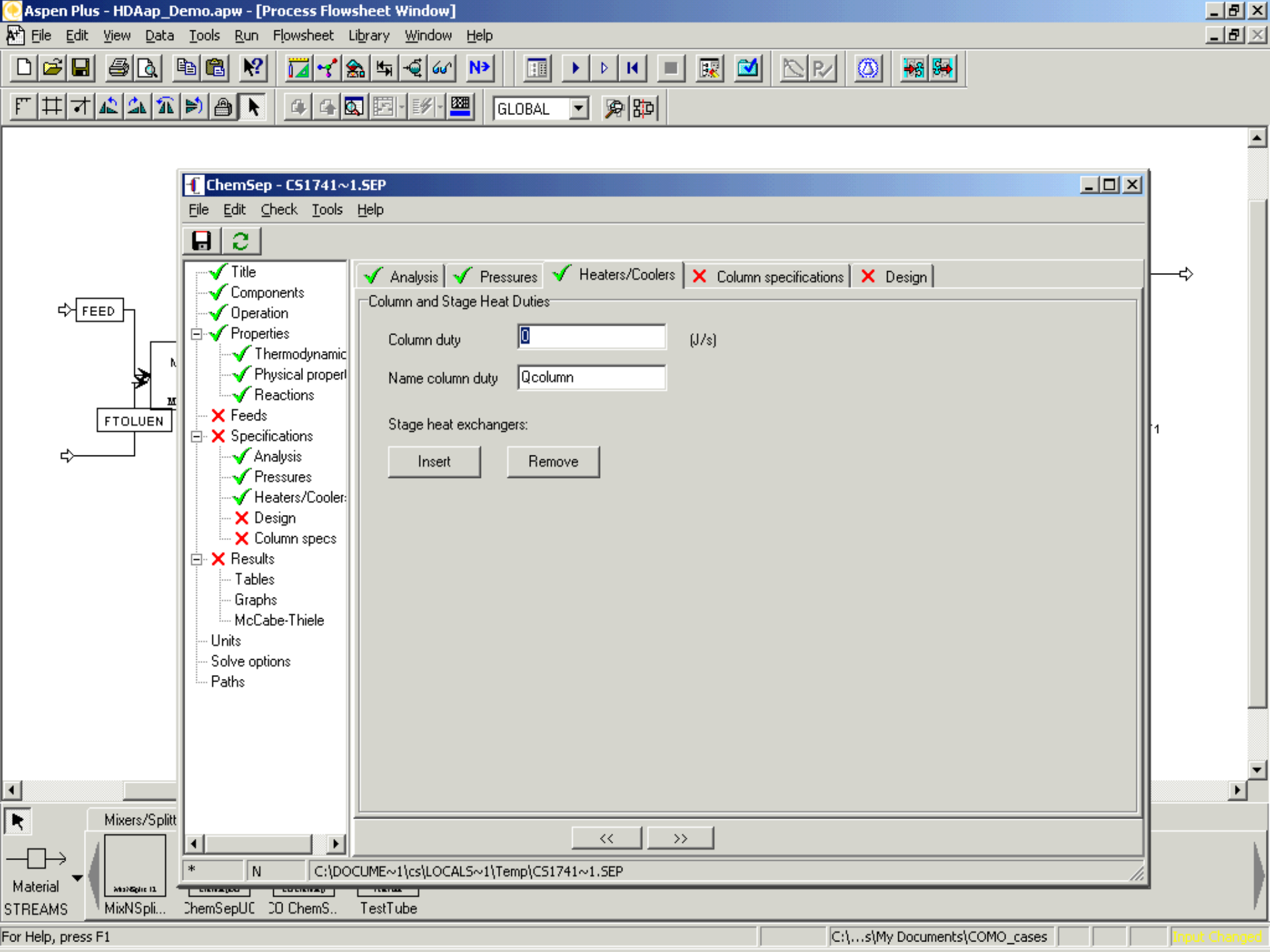
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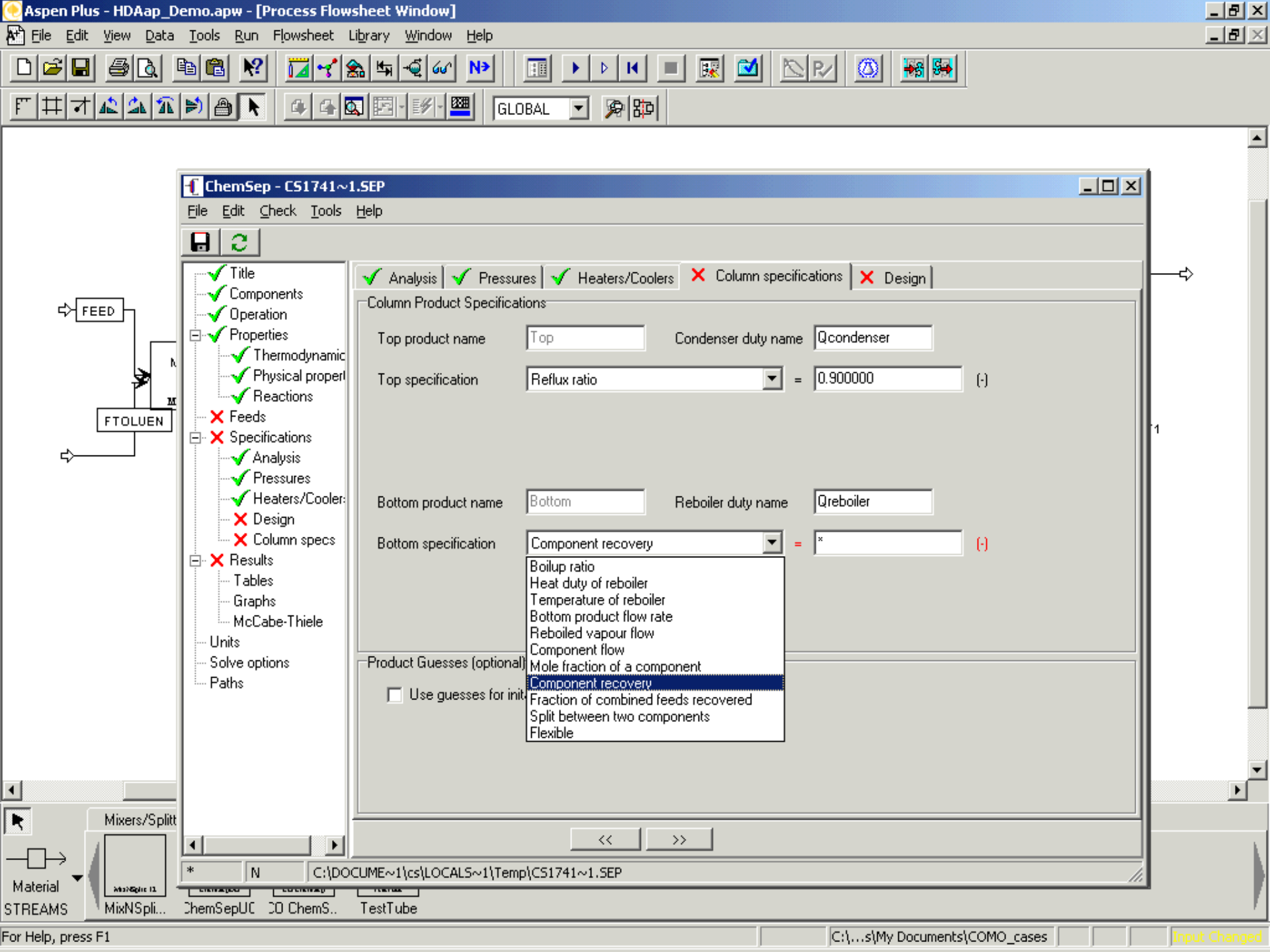
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Column specifications
Design
Column Product Specifications
Top product name
Top
Condenser duty name
Qcondenser
Top specification
Reflux ratio
=
0.900000
(-)
Bottom product name
Bottom
Reboiler duty name
Qreboiler
Bottom specification
Component recovery
=
*
(-)
Boilup ratio
Heat duty of reboiler
Temperature of reboiler
Bottom product flow rate
Reboiled vapour flow
Component flow
Mole fraction of a component
Component recovery
Fraction of combined feeds recovered
Split between two components
Flexible
Product Guesses (optional)
Use guesses for init
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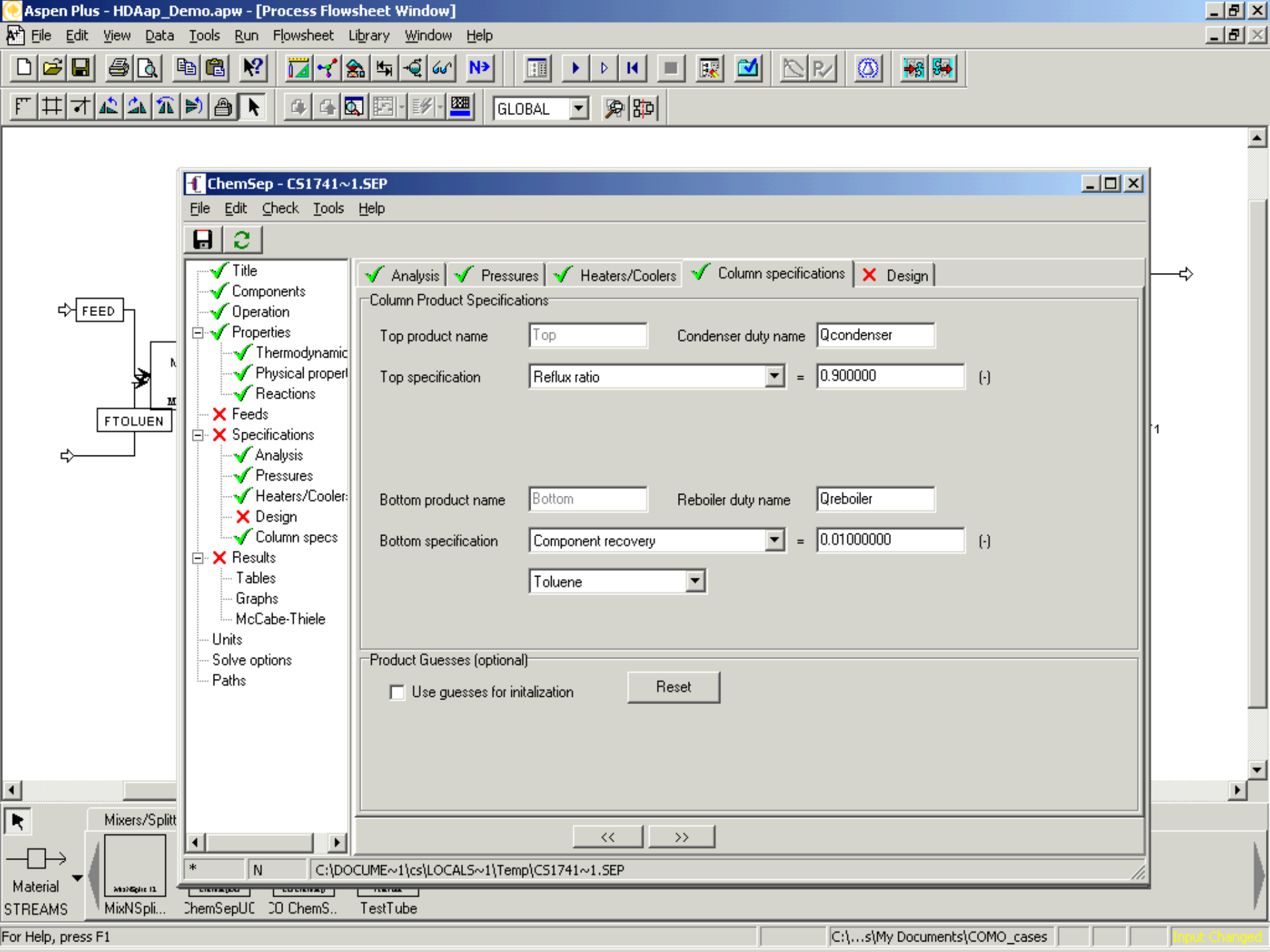
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Column specifications
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Column Product Specifications
Top product name
Top
Condenser duty name
Qcondenser
Top specification
Reflux ratio
=
0.900000
(-)
Bottom product name
Bottom
Reboiler duty name
Qreboiler
Bottom specification
Component recovery
=
0.01000000
(-)
Toluene
Product Guesses (optional)
Use guesses for initalization
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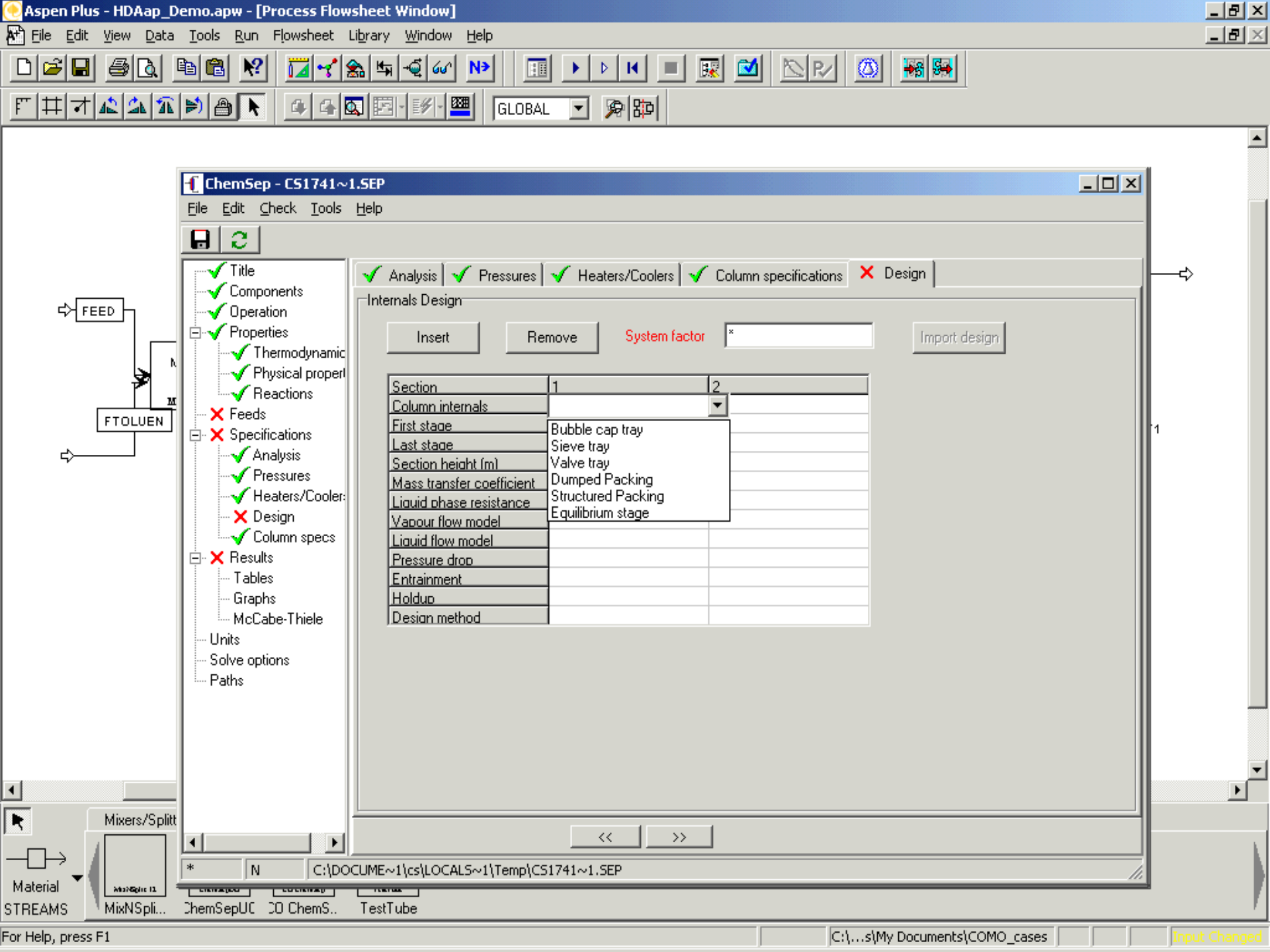
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Design
Internals Design
Insert
Remove
System factor
*
Import design
Section
1
2
Column internals
First stage
Last stage
Section height (m)
Mass transfer coefficient
Liquid phase resistance
Vapour flow model
Liquid flow model
Pressure drop
Entrainment
Holdup
Design method
Bubble cap tray
Sieve tray
Valve tray
Dumped Packing
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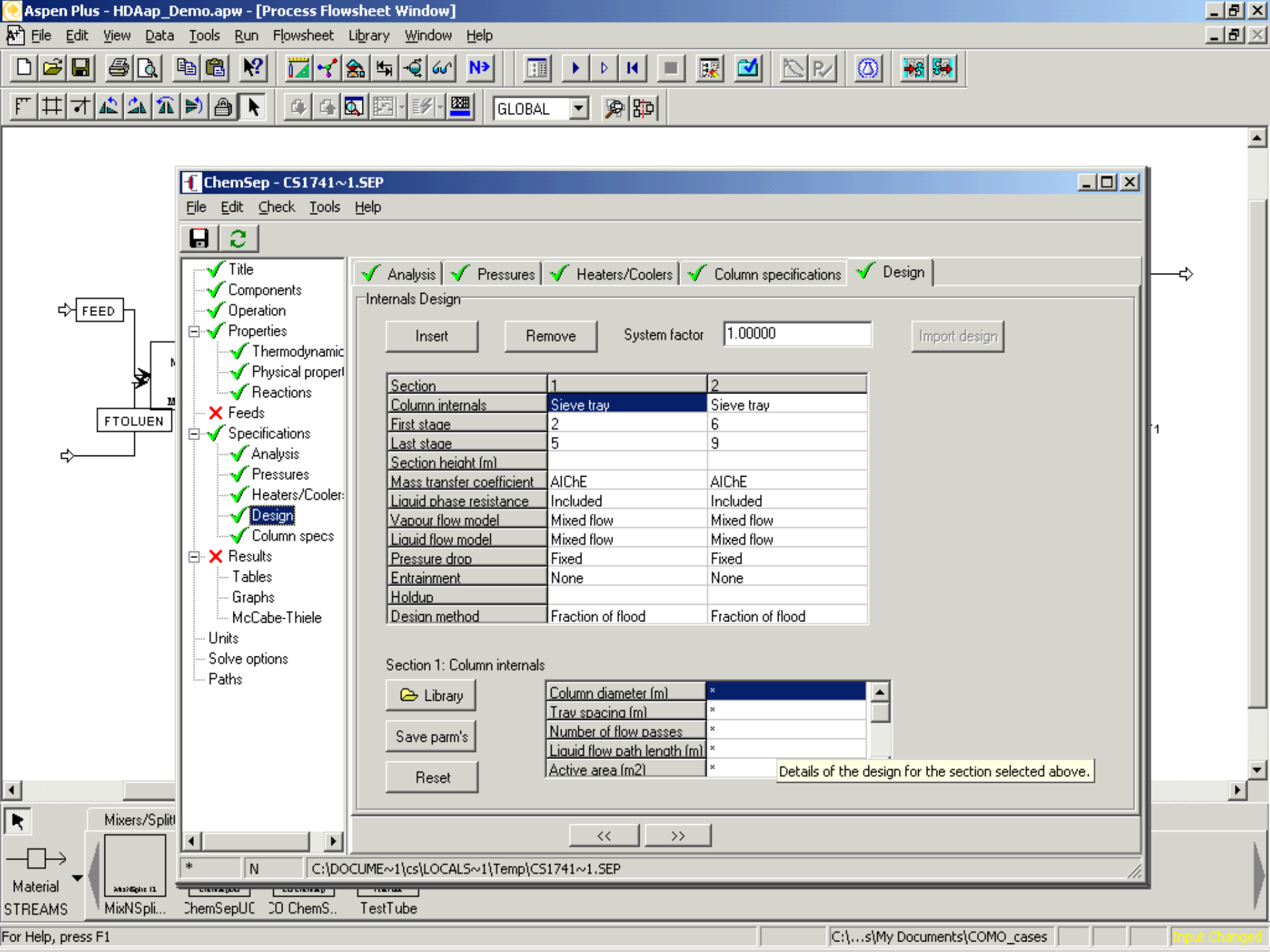
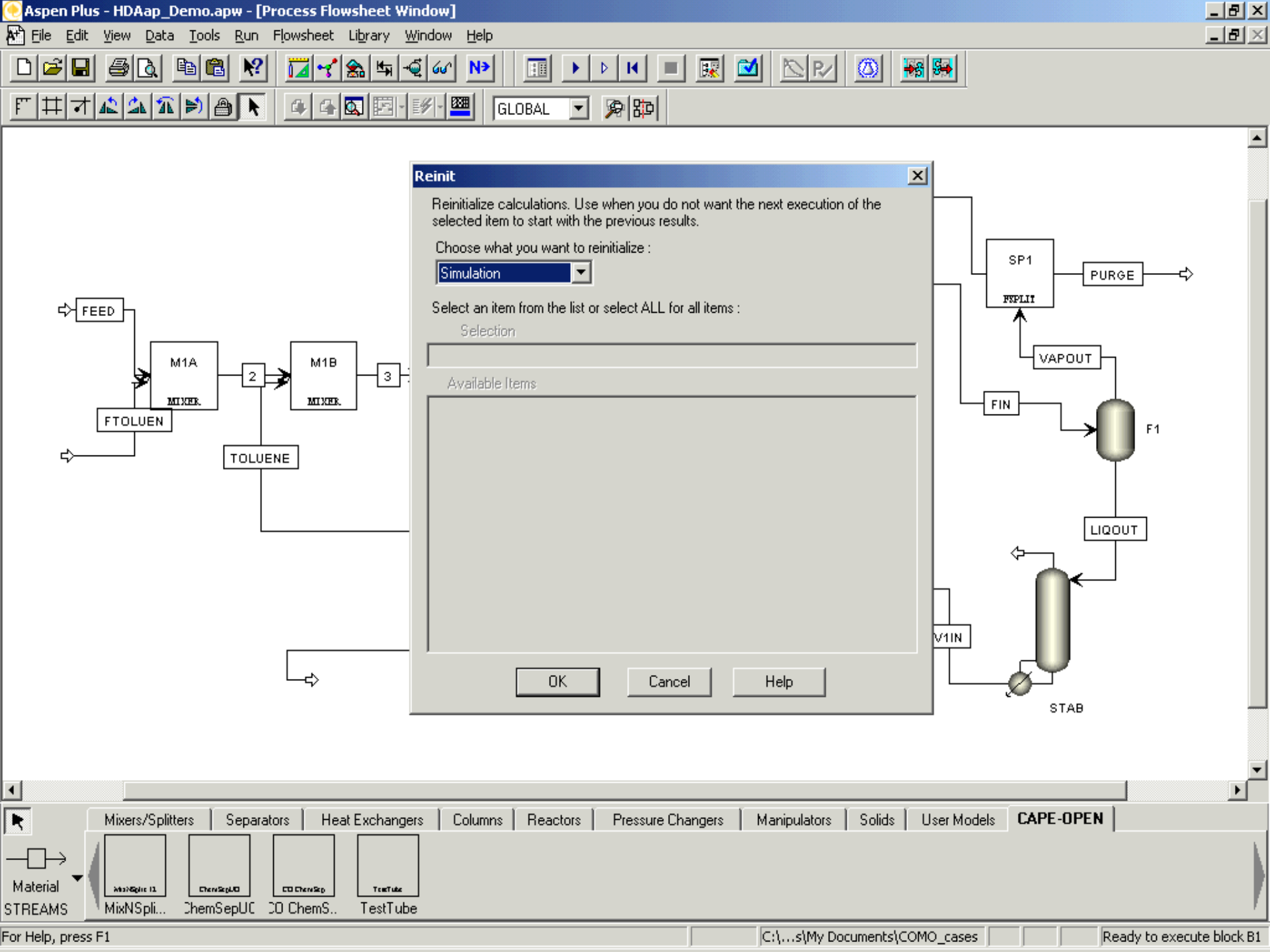

Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
FEED
FTOLUEN
ChemSep - CS1741~1.SEP
File Edit Check Tools Help
Title
Components
Operation
Properties
Thermodynamic
Physical properl
Reactions
Feeds
Specifications
Analysis
Pressures
Heaters/Cooler:
Design
Column specs
Results
Tables
Graphs
McCabe-Thiele
Units
Solve options
Paths
Analysis
Pressures
Heaters/Coolers
Column specifications
Design
Internals Design
Insert
Remove
System factor
1.00000
Import design
Section
1
2
Column internals
Sieve tray
Sieve tray
First stage
2
6
Last stage
5
9
Section height (m)
Mass transfer coefficient
AIChE
AIChE
Liquid phase resistance
Included
Included
Vapour flow model
Mixed flow
Mixed flow
Liquid flow model
Mixed flow
Mixed flow
Pressure drop
Fixed
Fixed
Entrainment
None
None
Holdup
Design method
Fraction of flood
Fraction of flood
Section 1: Column internals
Library
Save parm's
Reset
Column diameter (m)
Tray spacing (m)
Number of flow passes
Liquid flow path length (m)
Active area (m2)
Details of the design for the section selected above.
<<
>>
C:\DOCUME~1\cs\LOCALS~1\Temp\CS1741~1.SEP
Mixers/Split
Material
STREAMS
MixNSpli...
ChemSepUC
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases
Input Changed


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
Reinit
Reinitialize calculations. Use when you do not want the next execution of the selected item to start with the previous results.
Choose what you want to reinitialize :
Simulation
Select an item from the list or select ALL for all items :
Selection
Available Items
OK
Cancel
Help
FEED
M1A
MIXER
2
M1B
MIXER
3
FTOLUEN
TOLUENE
SP1
FSPLIT
PURGE
VAPOUT
FIN
F1
LIQOUT
V1IN
STAB
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
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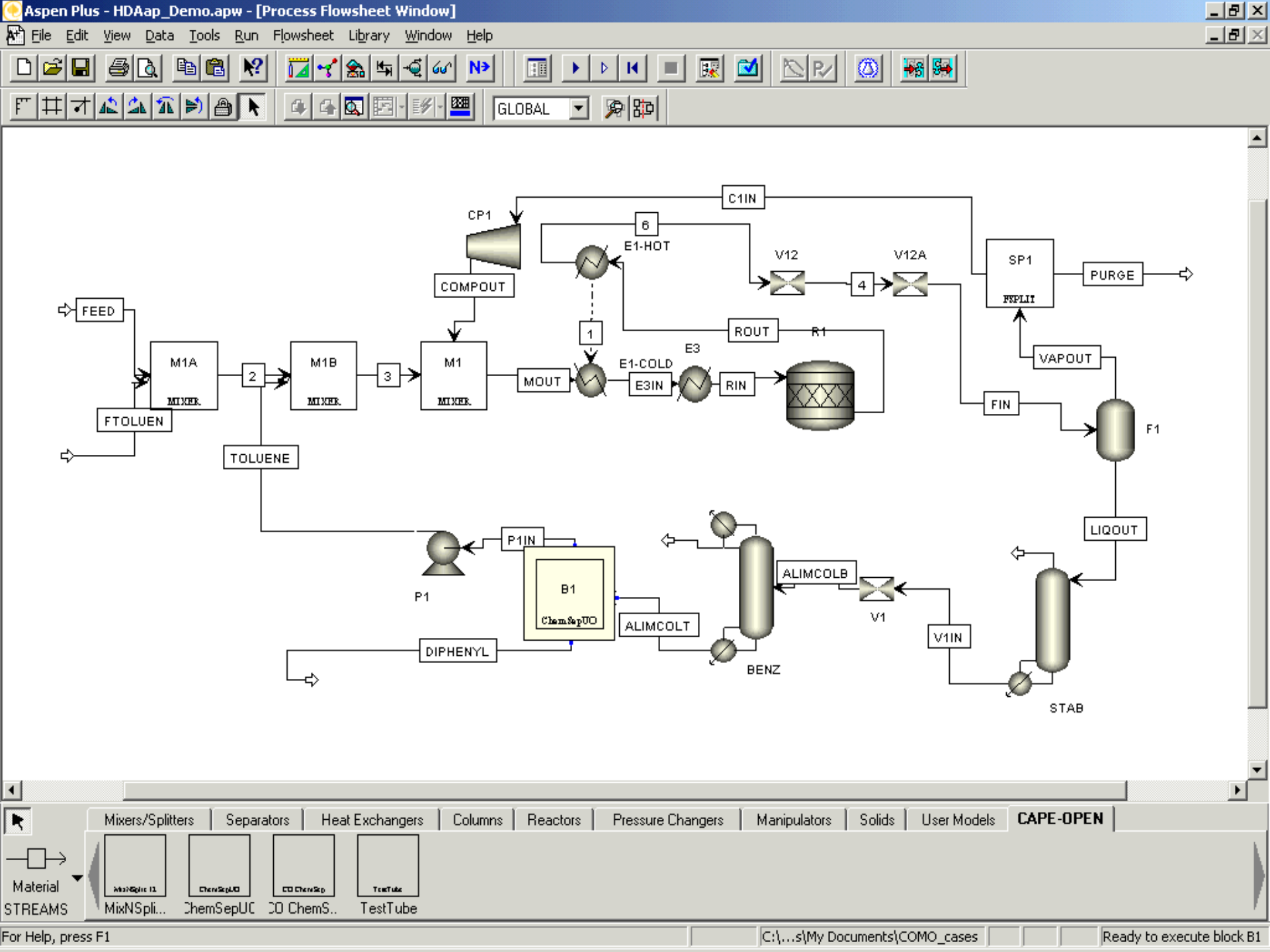
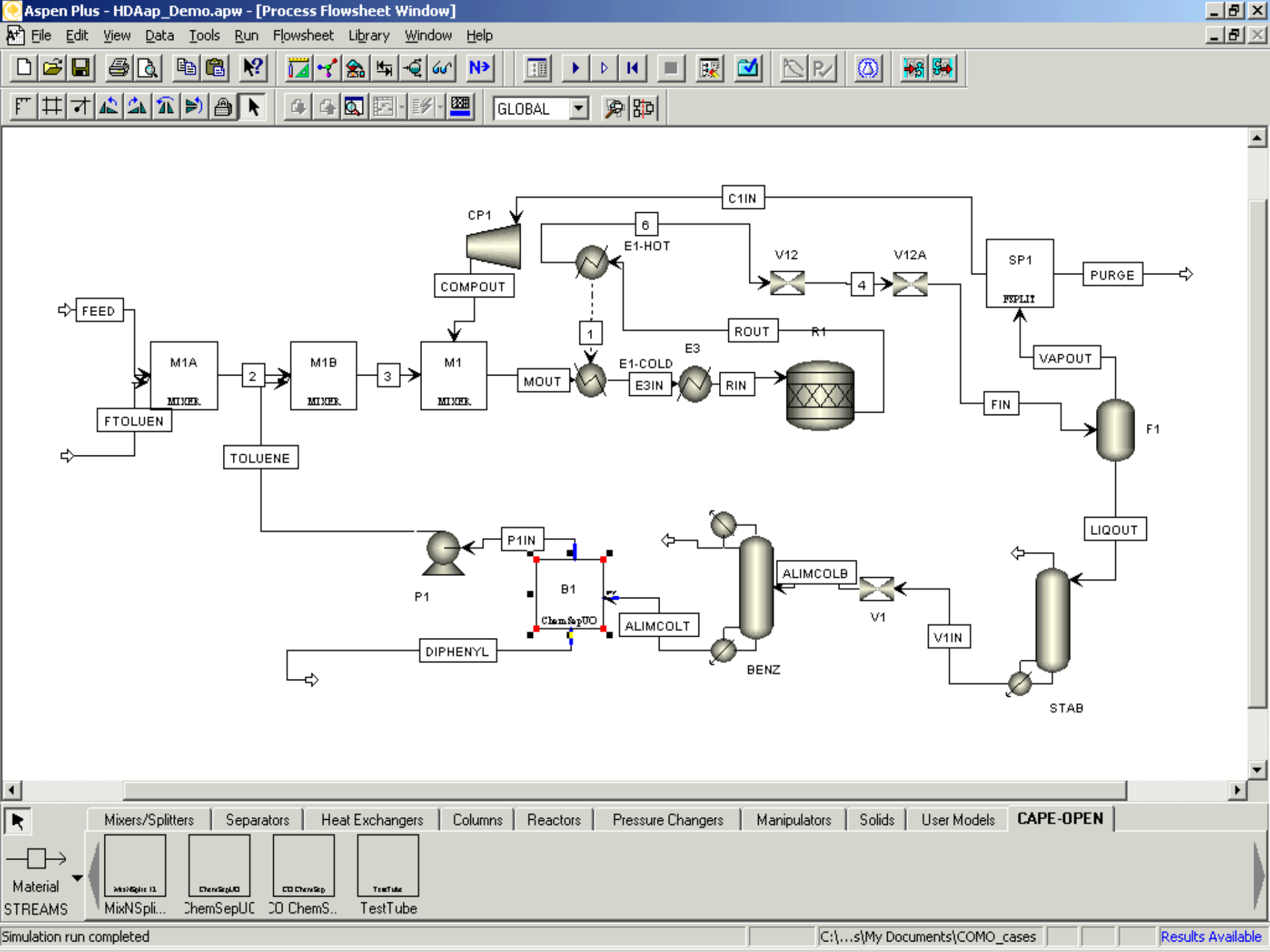
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases
Ready to execute block B1


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
C1IN
CP1
6
E1-HOT
V12
V12A
SP1
PURGE
COMPOUT
FEED
ROUT
R1
1
E3
E1-COLD
E3IN
RIN
VAPOUT
M1A
MIXER
2
M1B
MIXER
3
M1
MIXER
MOUT
FIN
F1
FTOLUEN
TOLUENE
LIQOUT
P1IN
P1
B1
ChemSepUO
ALIMCOLB
V1
ALIMCOLT
V1IN
DIPHENYL
BENZ
STAB
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases
Ready to execute block B1


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
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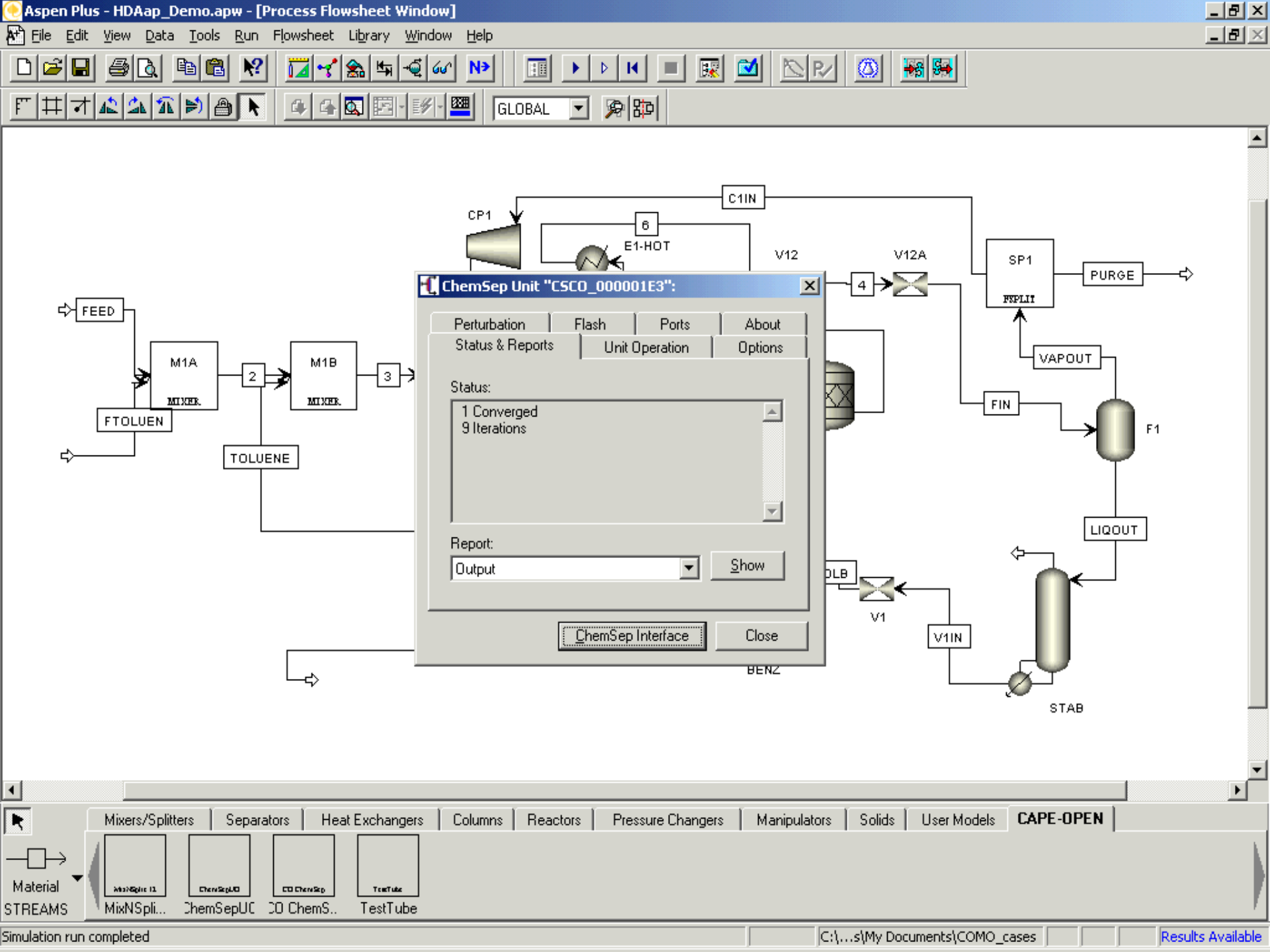
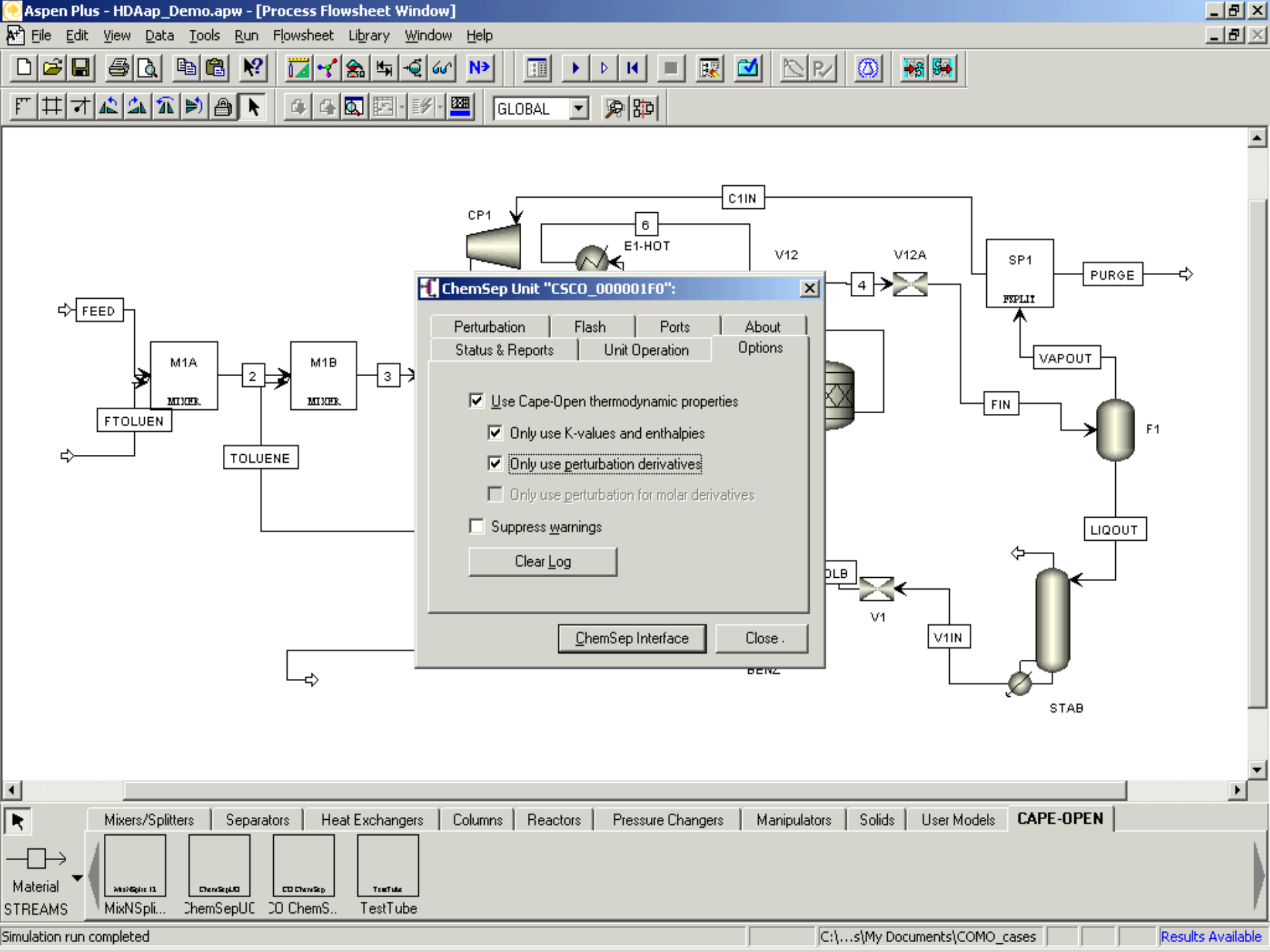
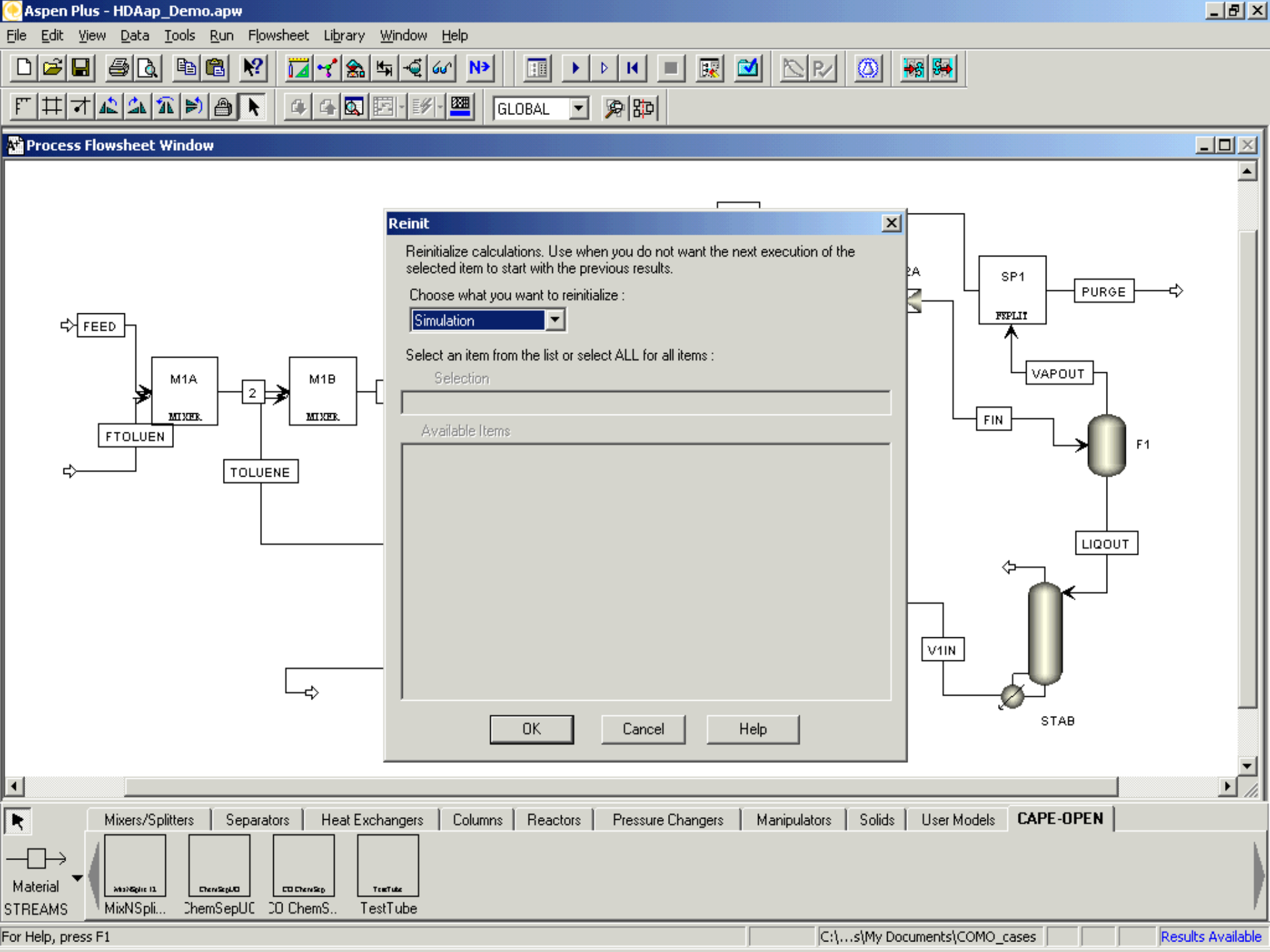
C1IN
CP1
6
E1-HOT
V12
V12A
SP1
PURGE
COMPOUT
FEED
ROUT
R1
1
E3
E1-COLD
E3IN
RIN
VAPOUT
M1A
MIXER
2
M1B
MIXER
3
M1
MIXER
MOUT
FIN
F1
FTOLUEN
TOLUENE
P1IN
LIQOUT
P1
B1
ChemSepUO
ALIMCOLB
V1
ALIMCOLT
V1IN
DIPHENYL
BENZ
STAB
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
Simulation run completed
C:\...s\My Documents\COMO_cases
Results Available


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
C1IN
CP1
6
E1-HOT
V12
V12A
SP1
PURGE
FEED
M1A
MIXER
2
M1B
MIXER
3
4
VAPOUR
FIN
F1
FTOLUEN
TOLUENE
LIQOUT
V1
V1IN
STAB
BENZ
ChemSep Unit "CSCO_000001E3":
Perturbation
Flash
Ports
About
Status & Reports
Unit Operation
Options
Status:
1 Converged
9 Iterations
Report:
Output
Show
ChemSep Interface
Close
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
Simulation run completed
C:\...s\My Documents\COMO_cases
Results Available


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
C1IN
CP1
6
E1-HOT
V12
V12A
SP1
PURGE
FEED
M1A
MIXER
2
M1B
MIXER
3
4
VAPOUT
FIN
F1
FTOLUEN
TOLUENE
LIQOUT
V1
V1IN
STAB
ChemSep Unit "CSCO_000001F0":
Perturbation
Flash
Ports
About
Status & Reports
Unit Operation
Options
Use Cape-Open thermodynamic properties
Only use K-values and enthalpies
Only use perturbation derivatives
Only use perturbation for molar derivatives
Suppress warnings
Clear Log
ChemSep Interface
Close
Mixers/Splitters
Separators
Heat Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
Simulation run completed
C:\...s\My Documents\COMO_cases
Results Available


Aspen Plus - HDAap_Demo.apw
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
Process Flowsheet Window
Reinit
Reinitialize calculations. Use when you do not want the next execution of the selected item to start with the previous results.
Choose what you want to reinitialize :
Simulation
Select an item from the list or select ALL for all items :
Selection
Available Items
OK
Cancel
Help
FEED
M1A
MIXER
2
M1B
MIXER
FTOLUEN
TOLUENE
SP1
FSPLIT
PURGE
VAPOUT
FIN
F1
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V1IN
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CO ChemS..
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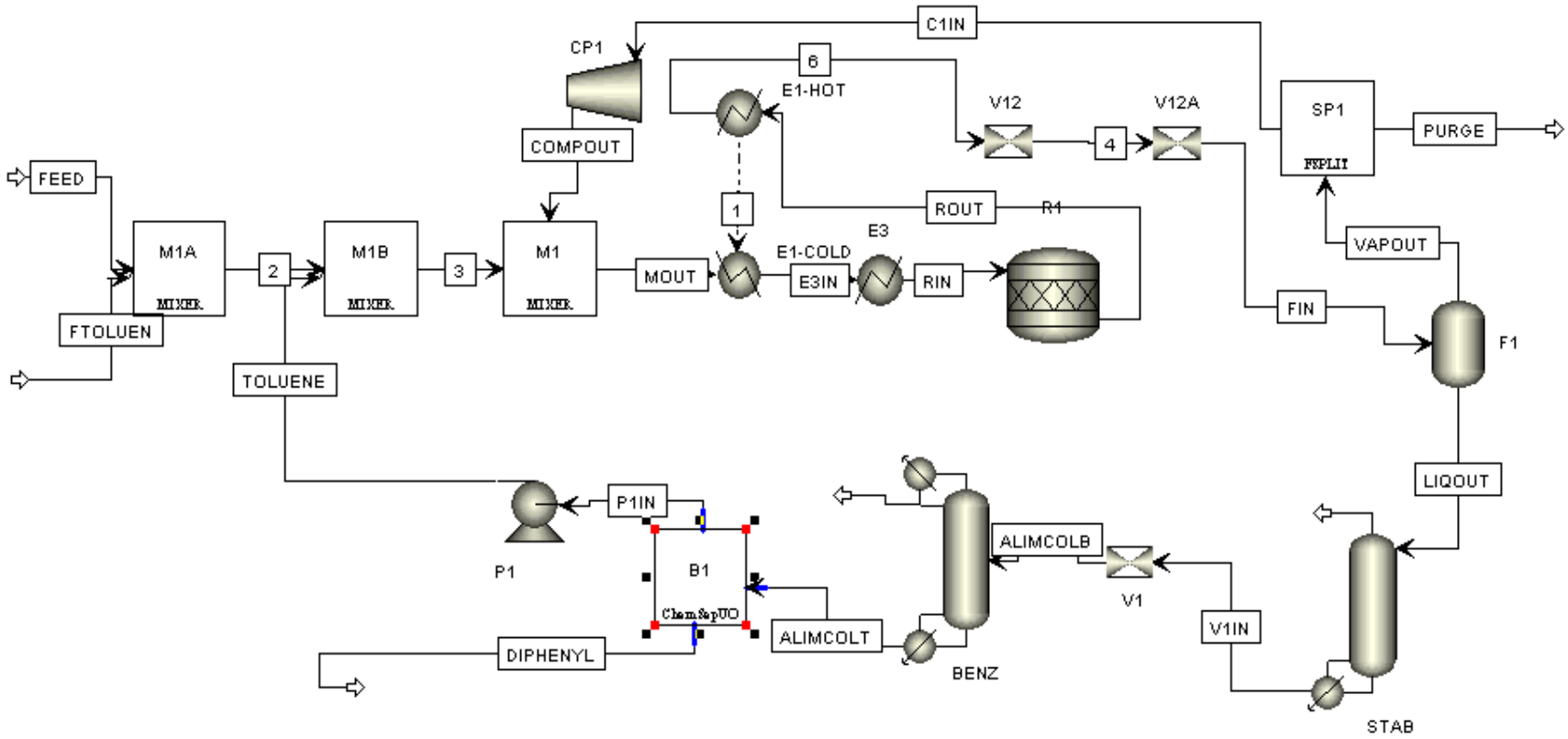
For Help, press F1
C:\...s\My Documents\COMO_cases
Results Available

Aspen Plus - HDAap_Demo.apw

File Edit View Data Tools Run Flowsheet Library Window Help

GLOBAL

Process Flowsheet Window

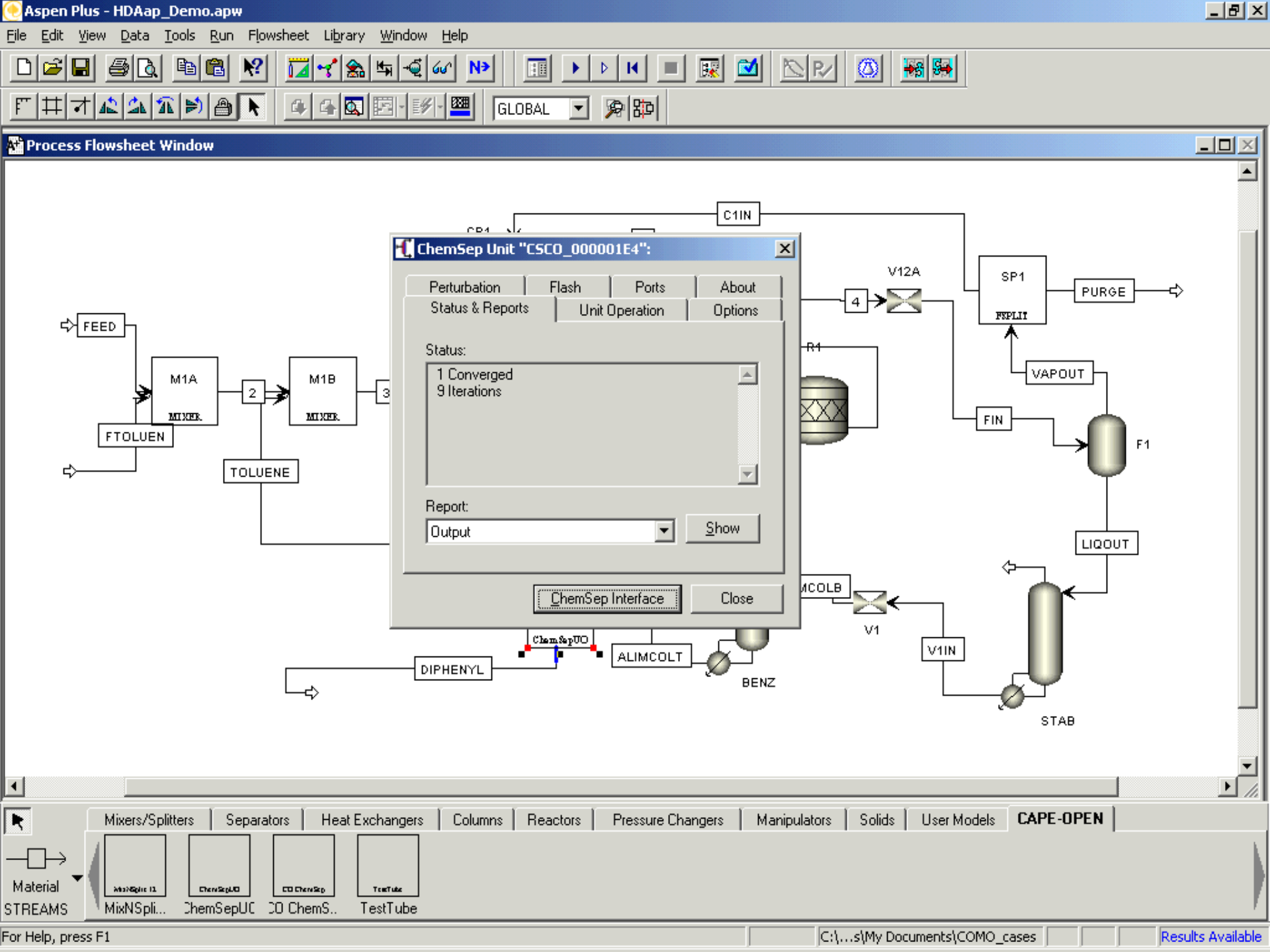


Mixers/Splitters | Separators | Heat Exchangers | Columns | Reactors | Pressure Changers | Manipulators | Solids | User Models | CAPE-OPEN

Material STREAMS

MixNSpli... ChemSepUC CO ChemS.. TestTube

For Help, press F1 | C:\...s\My Documents\COMO_cases | Results Available


Aspen Plus - HDAap_Demo.apw
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
Process Flowsheet Window
C1IN
ChemSep Unit "CSCO_000001E4":
Perturbation
Flash
Ports
About
Status & Reports
Unit Operation
Options
Status:
1 Converged
9 Iterations
Report:
Output
Show
ChemSep Interface
Close
V12A
SP1
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FEED
M1A
MIXER
2
M1B
MIXER
FTOLUEN
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F1
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V1
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STAB
ALIMCOLT
BENZ
DIPHENYL
Mixers/Splitters
Separators
Heat Exchangers
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Reactors
Pressure Changers
Manipulators
Solids
User Models
CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases
Results Available

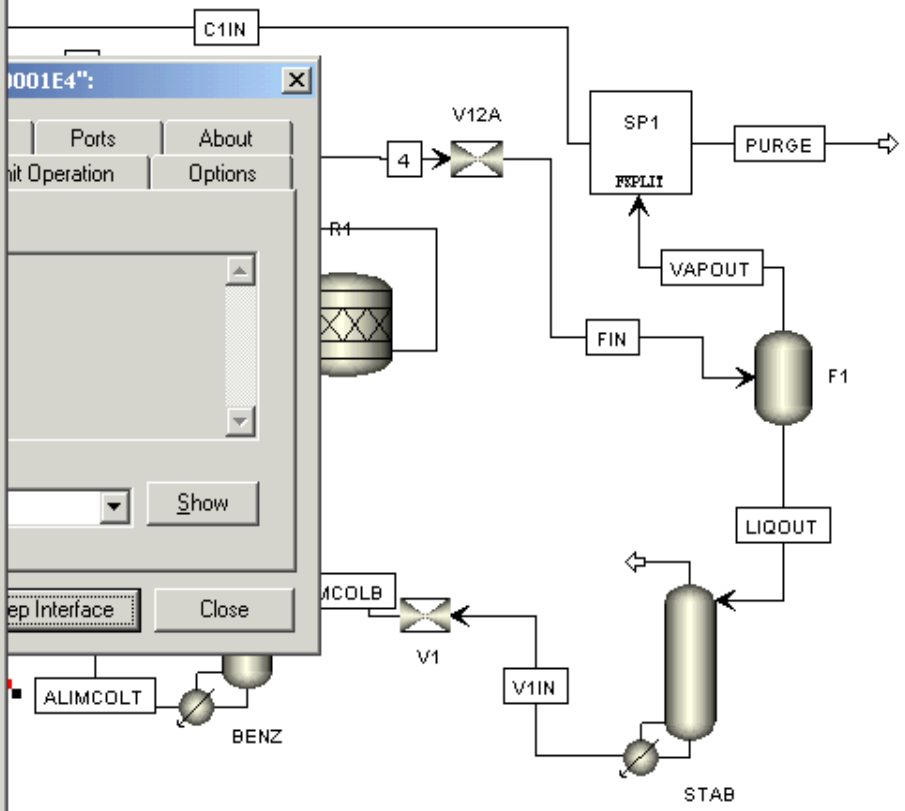
Output Report:

```
ChemSep (TM) - Neq2 v5.00s
Copyright(c) R.Taylor and H.A.Kooijman 1991-2005
Checking data file C:\DOCUME~1\cs\LOCALS~1\Temp\CS1I
Cape Open unit name: CSCO_000001E4
Cape-Open unit id: CSCO_000001E4
Cape Open Initialized
Cape Open Thermodynamic-properties enabled
Reading component property data
Reading thermodynamic property options
Reading physical property options
Reading thermodynamic property data
EOS parameters missing - set to zero
Reading column specifications
Checking Component Data
 Hydrogen
 Methane
 Benzene
 Toluene
 Biphenyl
Determining feed conditions
Reading initial temperature profiles
Reading initial composition profiles
Reading column design data
Design mode ON
Reading user data
Starting Newtons method
Ctrl-Break will terminate execution

      Iteration                Error

         0                     4.2578E-01
         1                     1.4244E-02
         2                     5.8413E-03
         3                     2.7507E-03
         4                     1.5641E-03
         5                     8.1047E-04
         6                     4.2911E-04
         7                     2.2700E-04
         8                     1.2014E-04
         9                     6.3560E-05
Convergence obtained in 9 iterations

run time: 3.9 seconds
```



Pressure Changers | Manipulators | Solids | User Models | CAPE-OPEN

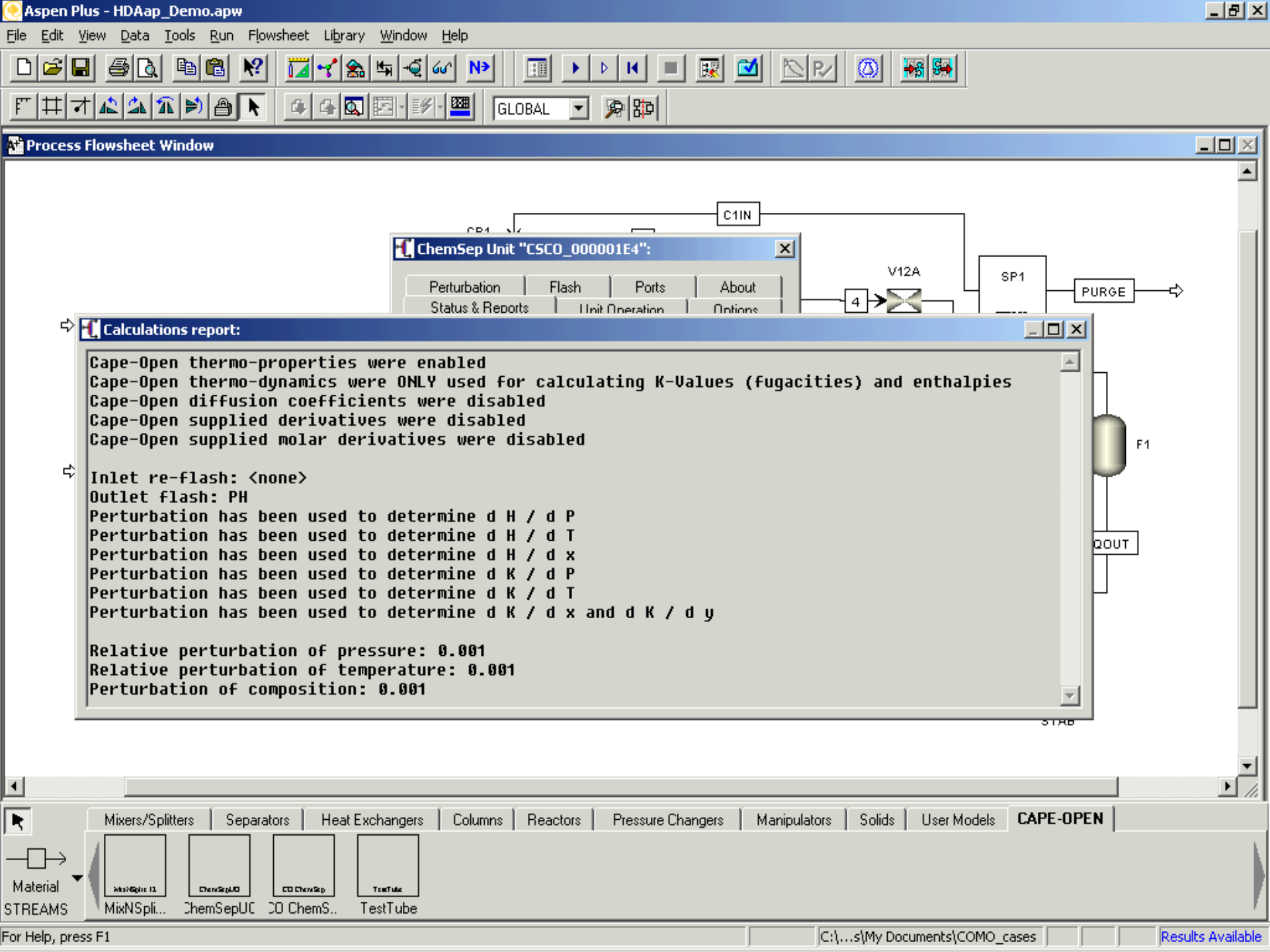
Material STREAMS

MixNSpli... ChemSepUC CO ChemS.. TestTube

For Help, press F1

C:\...s\My Documents\COMO_cases

Results Available


Aspen Plus - HDAap_Demo.apw
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
Process Flowsheet Window
C1IN
ChemSep Unit "CSCO_000001E4":
Perturbation Flash Ports About
Status & Reports Unit Operation Options
V12A
SP1
PURGE
4
Calculations report:
Cape-Open thermo-properties were enabled
Cape-Open thermo-dynamics were ONLY used for calculating K-Values (fugacities) and enthalpies
Cape-Open diffusion coefficients were disabled
Cape-Open supplied derivatives were disabled
Cape-Open supplied molar derivatives were disabled
Inlet re-flash: <none>
Outlet flash: PH
Perturbation has been used to determine d H / d P
Perturbation has been used to determine d H / d T
Perturbation has been used to determine d H / d x
Perturbation has been used to determine d K / d P
Perturbation has been used to determine d K / d T
Perturbation has been used to determine d K / d x and d K / d y
Relative perturbation of pressure: 0.001
Relative perturbation of temperature: 0.001
Perturbation of composition: 0.001
F1
QOUT
Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models CAPE-OPEN
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases
Results Available

Log report:

```
creating unit operation...
detected Aspen COSE
initializing...
performing Edit()...
initializing as new file...
using sep file C:\DOCUME~1\cs\LOCALS~1\Temp\CSCO_000001E4.sep
starting Chemsep: "c:\Documents and Settings\cs\My Documents\ChemSep\bin\wincs.exe" /Cape-Open /kpld /new="C:\DOCUME
fixing components in Sep file...
starting Chemsep: "c:\Documents and Settings\cs\My Documents\ChemSep\bin\wincs.exe" /Cape-Open /kpld /cc C:\DOCUME~1
performing Edit()...
starting Chemsep: "c:\Documents and Settings\cs\My Documents\ChemSep\bin\wincs.exe" /Cape-Open /kpld C:\DOCUME~1\cs\
connecting port BottomProduct to stream
connecting port TopProduct to stream
connecting port Feed_stage6 to stream
performing Edit()...
starting Chemsep: "c:\Documents and Settings\cs\My Documents\ChemSep\bin\wincs.exe" /Cape-Open /kpld C:\DOCUME~1\cs\
disconnecting port Feed_stage6 from stream ALIMCOLT
connecting port Feed_stage6 to stream
disconnecting port TopProduct from stream P1IN
connecting port TopProduct to stream
disconnecting port BottomProduct from stream DIPHENYL
connecting port BottomProduct to stream
disconnecting port Feed_stage6 from stream ALIMCOLT
connecting port Feed_stage6 to stream
disconnecting port TopProduct from stream P1IN
connecting port TopProduct to stream
disconnecting port BottomProduct from stream DIPHENYL
connecting port BottomProduct to stream
performing Edit()...
starting calculate at 09/02/2005 / 15:31:46
 connected to material object Feed_stage6:
405.386556946 Temperature
103421.3595 Pressure
0 Vapour fraction
0 Component 1 flow
0 Component 2 flow
2.22449814001e-007 Component 3 flow
0.000747230278751 Component 4 flow
0.00058640770421 Component 5 flow
run time: 17 seconds
  1 Converged
 37 Iterations
```

Material STREAMS

MixNSpli... ChemSepUC CO ChemS.. TestTube

For Help, press F1

C:\...s\My Documents\COMO_cases

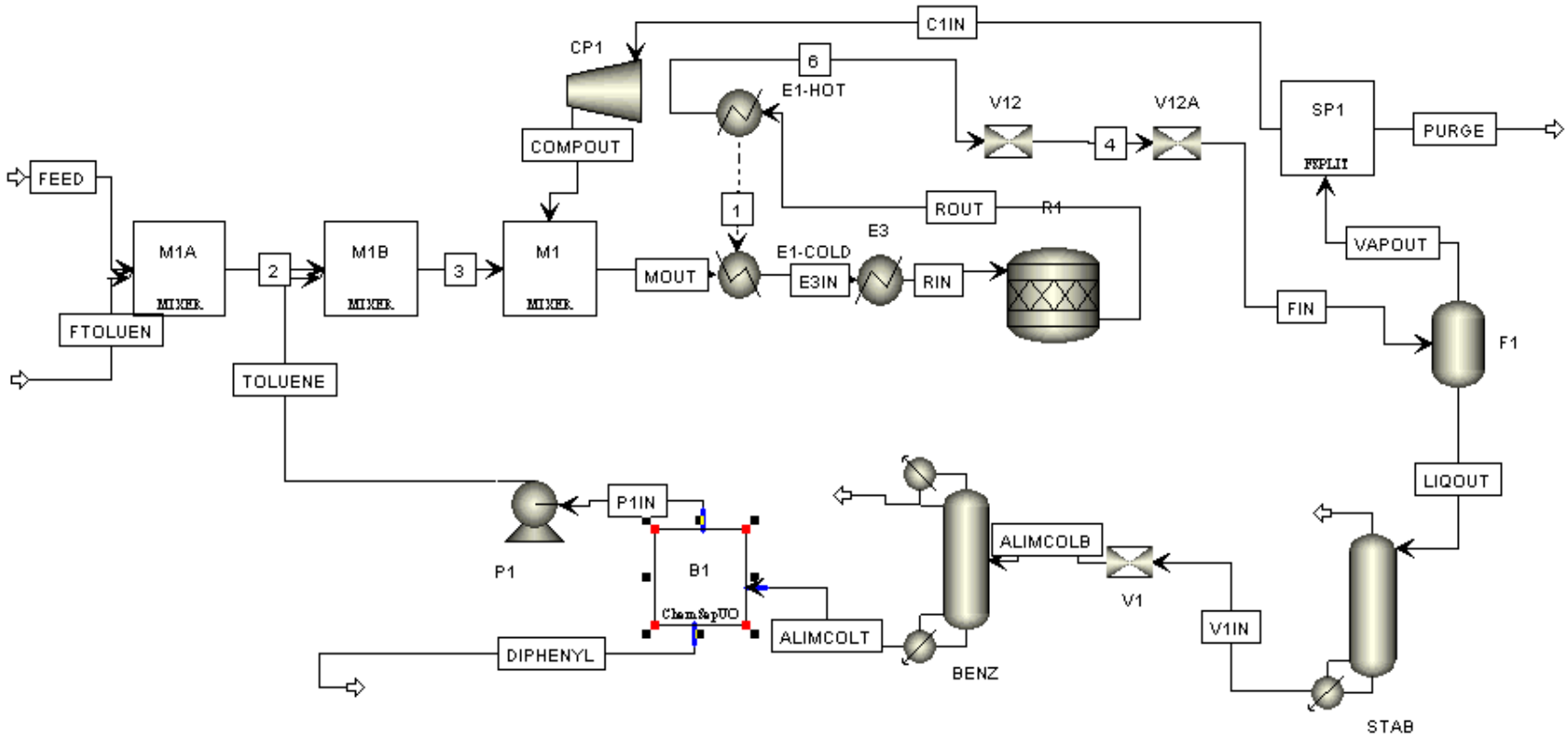
Results Available

Aspen Plus - HDAap_Demo.apw

File Edit View Data Tools Run Flowsheet Library Window Help

GLOBAL

Process Flowsheet Window



Mixers/Splitters | Separators | Heat Exchangers | Columns | Reactors | Pressure Changers | Manipulators | Solids | User Models | CAPE-OPEN

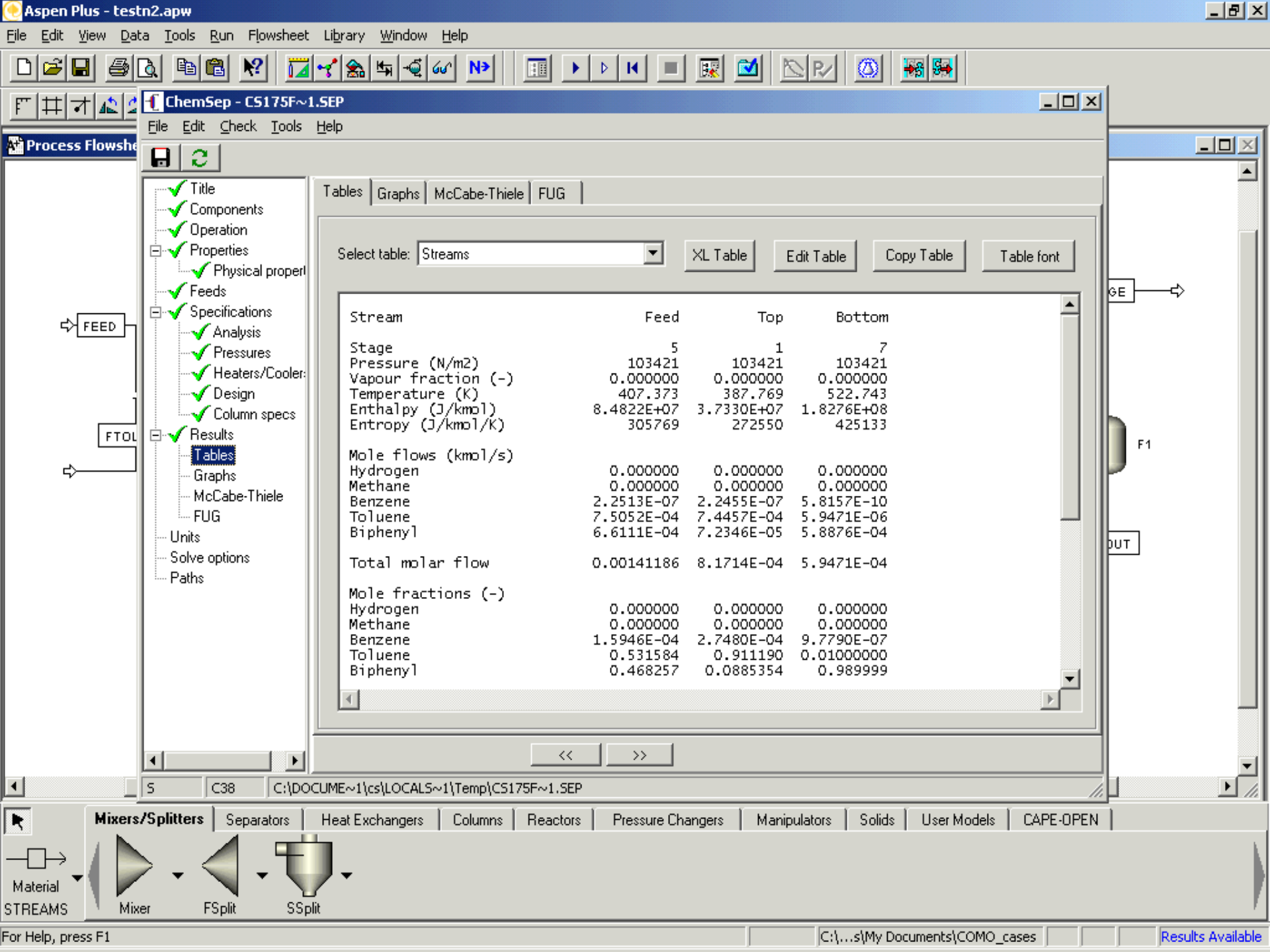
Material STREAMS

MixNSpli... ChemSepUC CO ChemS.. TestTube

Simulation run completed

C:\...s\My Documents\COMO_cases

Results Available


Aspen Plus - testn2.apw
File Edit View Data Tools Run Flowsheet Library Window Help
ChemSep - CS175F~1.SEP
File Edit Check Tools Help
Title
Components
Operation
Properties
Physical properl
Feeds
Specifications
Analysis
Pressures
Heaters/Cooler:
Design
Column specs
Results
Tables
Graphs
McCabe-Thiele
FUG
Units
Solve options
Paths
Tables Graphs McCabe-Thiele FUG
Select table: Streams
XL Table
Edit Table
Copy Table
Table font
Stream Feed Top Bottom
Stage 5 1 7
Pressure (N/m2) 103421 103421 103421
Vapour fraction (-) 0.000000 0.000000 0.000000
Temperature (K) 407.373 387.769 522.743
Enthalpy (J/kmol) 8.4822E+07 3.7330E+07 1.8276E+08
Entropy (J/kmol/K) 305769 272550 425133
Mole flows (kmol/s)
Hydrogen 0.000000 0.000000 0.000000
Methane 0.000000 0.000000 0.000000
Benzene 2.2513E-07 2.2455E-07 5.8157E-10
Toluene 7.5052E-04 7.4457E-04 5.9471E-06
Biphenyl 6.6111E-04 7.2346E-05 5.8876E-04
Total molar flow 0.00141186 8.1714E-04 5.9471E-04
Mole fractions (-)
Hydrogen 0.000000 0.000000 0.000000
Methane 0.000000 0.000000 0.000000
Benzene 1.5946E-04 2.7480E-04 9.7790E-07
Toluene 0.531584 0.911190 0.01000000
Biphenyl 0.468257 0.0885354 0.989999
<< >>
S C38 C:\DOCUME~1\cs\LOCALS~1\Temp\CS175F~1.SEP
FEED
FTOL
GE
F1
OUT
Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models CAPE-OPEN
Material STREAMS
Mixer
FSplit
SSplit
For Help, press F1
C:\...s\My Documents\COMO_cases
Results Available

Aspen Plus - testn2.apw

File Edit View Data Tools Run Flowsheet Library Window Help

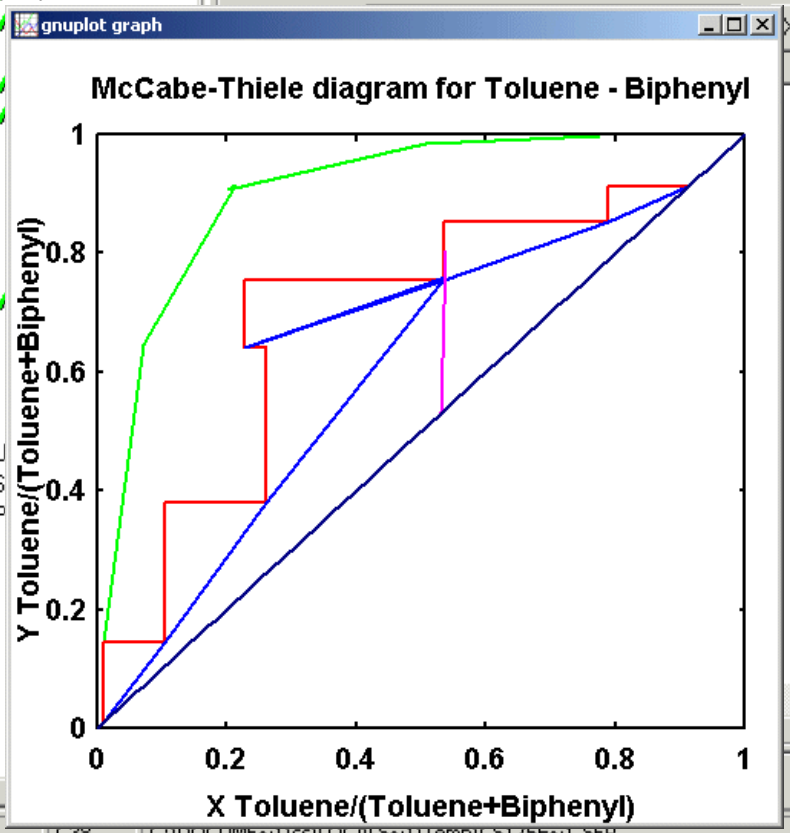
ChemSep - CS175F~1.SEP

File Edit Check Tools Help

Title
Components
Operation

Tables | Graphs | McCabe-Thiele | FUG

gnuplot graph



XL Table

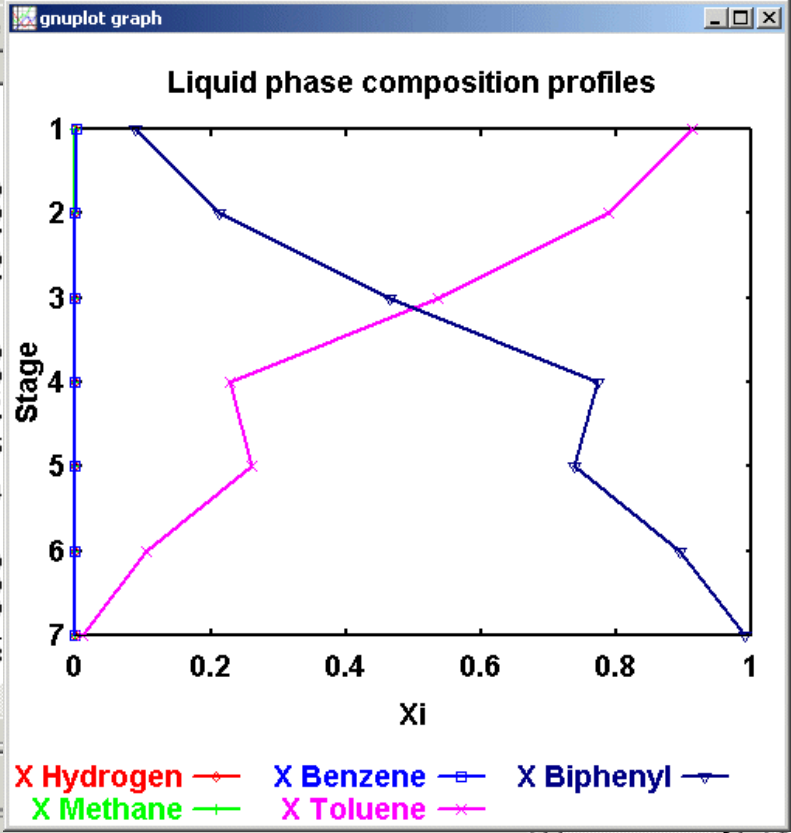
10
0.00
387
3.7330
27

0.00
0.00
2.2455
7.4457
7.2346

8.1714

0.00
0.00
2.7480
0.91
0.088

gnuplot graph



FEED

FTOL

Mixers/Splitters | Separators | Heat Exchangers | Columns | Reactors | Pressure Changers | Manipulators | Solids | User Models | CAPE-OPEN

Material STREAMS

Mixer FSplit SSplit

For Help, press F1

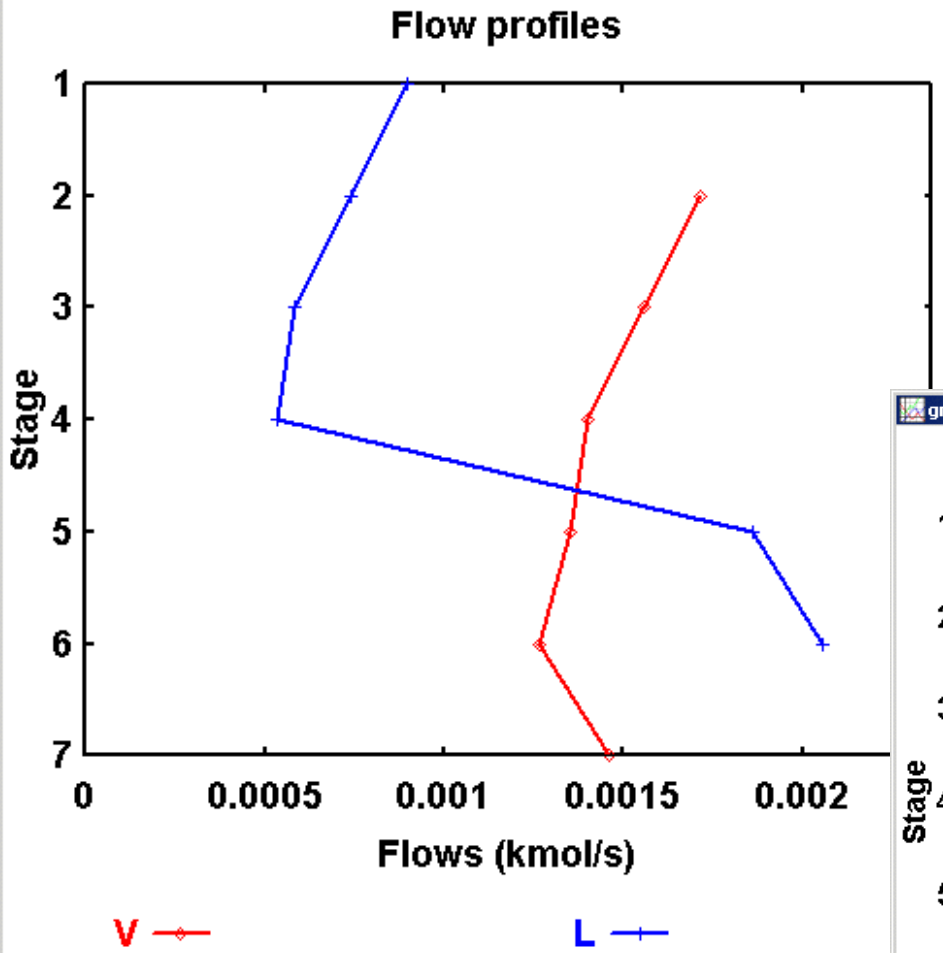
C:\...s\My Documents\COMO_cases

Results Available

Aspen Plus - testn2.apw

File Edit View Da

gnuplot graph



Process Flowshe

FEED

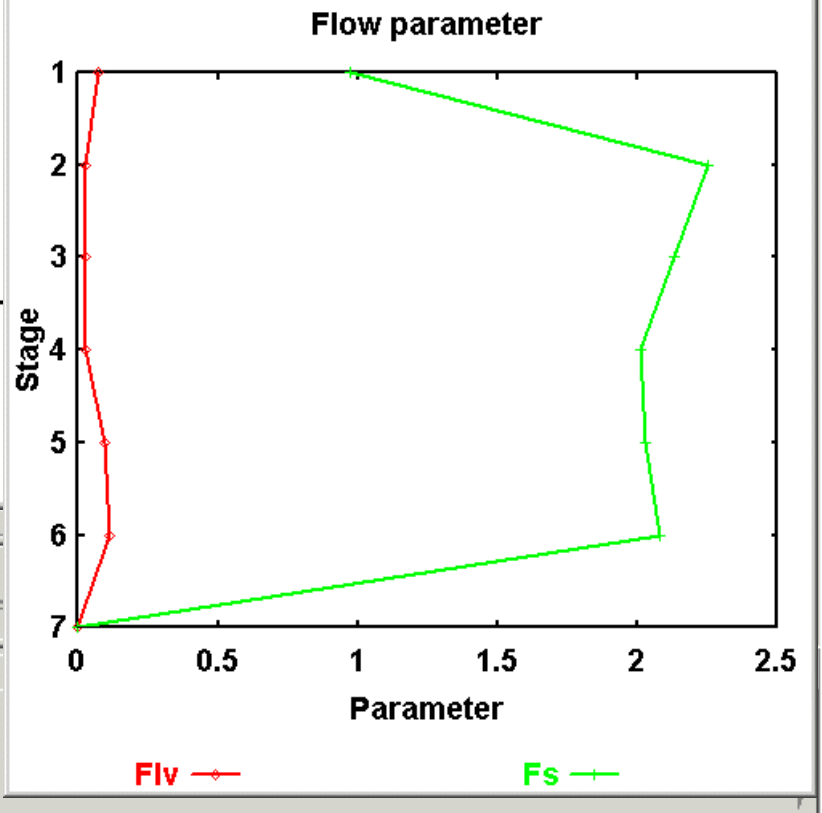
FTOL

Edit Table | Copy Table | Table font

Bottom

GE

gnuplot graph



<< >>

S C38 C:\DOCUME~1\cs\LOCALS~1\Temp\CS175F~1.SEP

Mixers/Splitters | Separators | Heat Exchangers | Columns | Reactors | Pressure Changers

Material STREAMS

Mixer FSplit SSplit

For Help, press F1

C:\...s\My Documents\COMO_cases

Results Available

CO ChemSep: Issues

- Using CAPE-OPEN thermo greatly increases run time.
- Most simulation packages do not provide binary Maxwell-Stefan diffusion coefficients.
- SMILES and UNIFAC structures should be CO property constants.

What is ChemSep Now?

- More than just a distillation column simulator.
- Features the original nonequilibrium column model.
- Functions with your favorite process flowsheet simulator
  - as long as it is CAPE-OPEN compliant.
- Tested with Aspen Plus, HYSYS, COCO(?).

COCO - Flowsheet1.fsd

File Edit Flowsheet View Window Help

Flowsheet1

Flowsheet1.fsd

ChemSepU...

Unit operation ChemSepUO_2:

Status | Edit | Ports | Info

Parameter	Value
GUIArguments	/kpld
UseCOSEThermo	FALSE
UseCOSEDiffusionCoefficients	FALSE
UsePerturbedDerivativesOnly	FALSE
UsePerturbed_ddX	FALSE
SuppressWarnings	FALSE
RelativePerturbationTemperature	0.001
RelativePerturbationPressure	0.001
PerturbationComposition	0.001
InletReflash	<none>
OutletFlash	TP
UseOnlyKValuesAndEnthalpyFromCOSE	FALSE
TryUsingRestartData	TRUE

Show GUI

ChemSep - C5F043~1.SEP

File Edit Check Tools Help

- Title
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  - Physical properl
  - Reactions
- Feeds
- Specifications
  - Analysis
  - Pressures
  - Heaters/Cooler:
  - Design
  - Column specs
- Results
  - Tables
  - Graphs
  - McCabe-Thiele
  - FUG
- Units
- Solve options
- Paths

Tables | Graphs | McCabe-Thiele | FUG

Auto-select key comp's

Key component 1: Propane

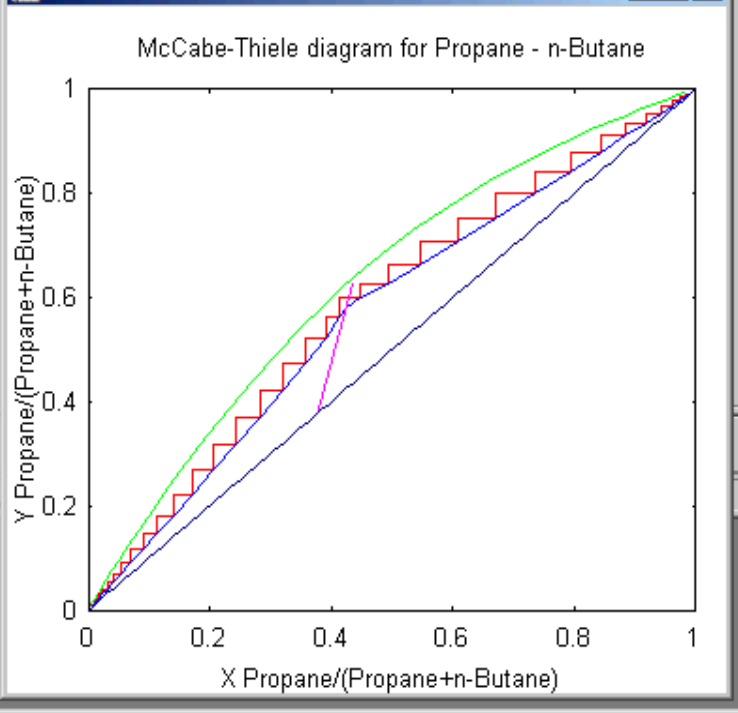
Key component 2: n-Butane

Display

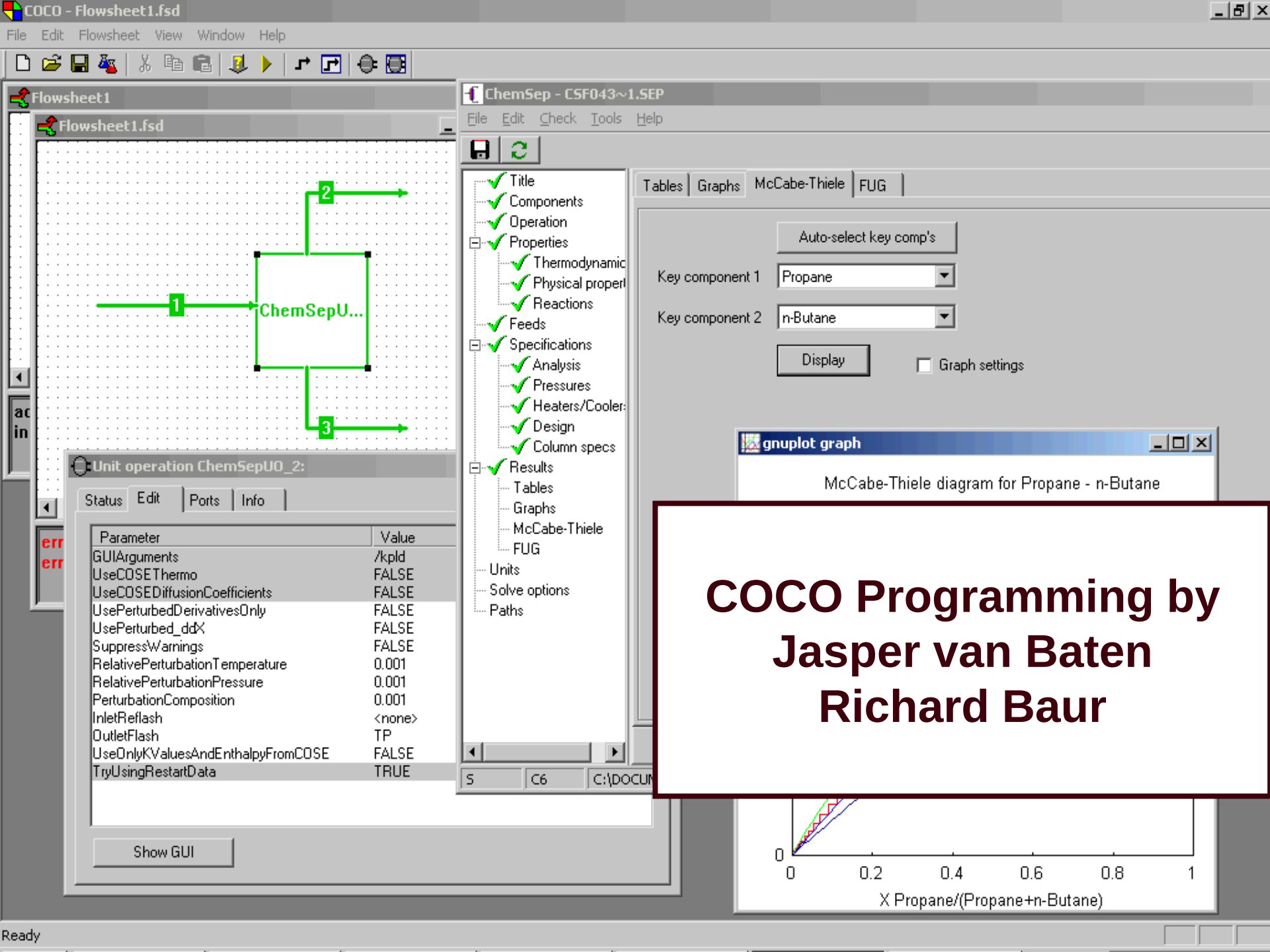
Graph settings

S | C6 | C:\DOCUME~1\richard\

gnuplot graph



Ready


COCO - Flowsheet1.fsd
File Edit Flowsheet View Window Help
Flowsheet1
Flowsheet1.fsd
ChemSepU...
Unit operation ChemSepUO_2:
Status Edit Ports Info
Parameter Value
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Auto-select key comp's
Key component 1 Propane
Key component 2 n-Butane
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gnuplot graph
McCabe-Thiele diagram for Propane - n-Butane
0
0 0.2 0.4 0.6 0.8 1
X Propane/(Propane+n-Butane)
COCO Programming by
Jasper van Baten
Richard Baur
Ready

What's next for CO ChemSep?

- Three-phase nonequilibrium model
- Flow models
- Reactive distillation

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