AVEVA PI WORLD

Distillation Column Convergence in AVEVA™ PRO/II™ Simulation

E-4-S/L

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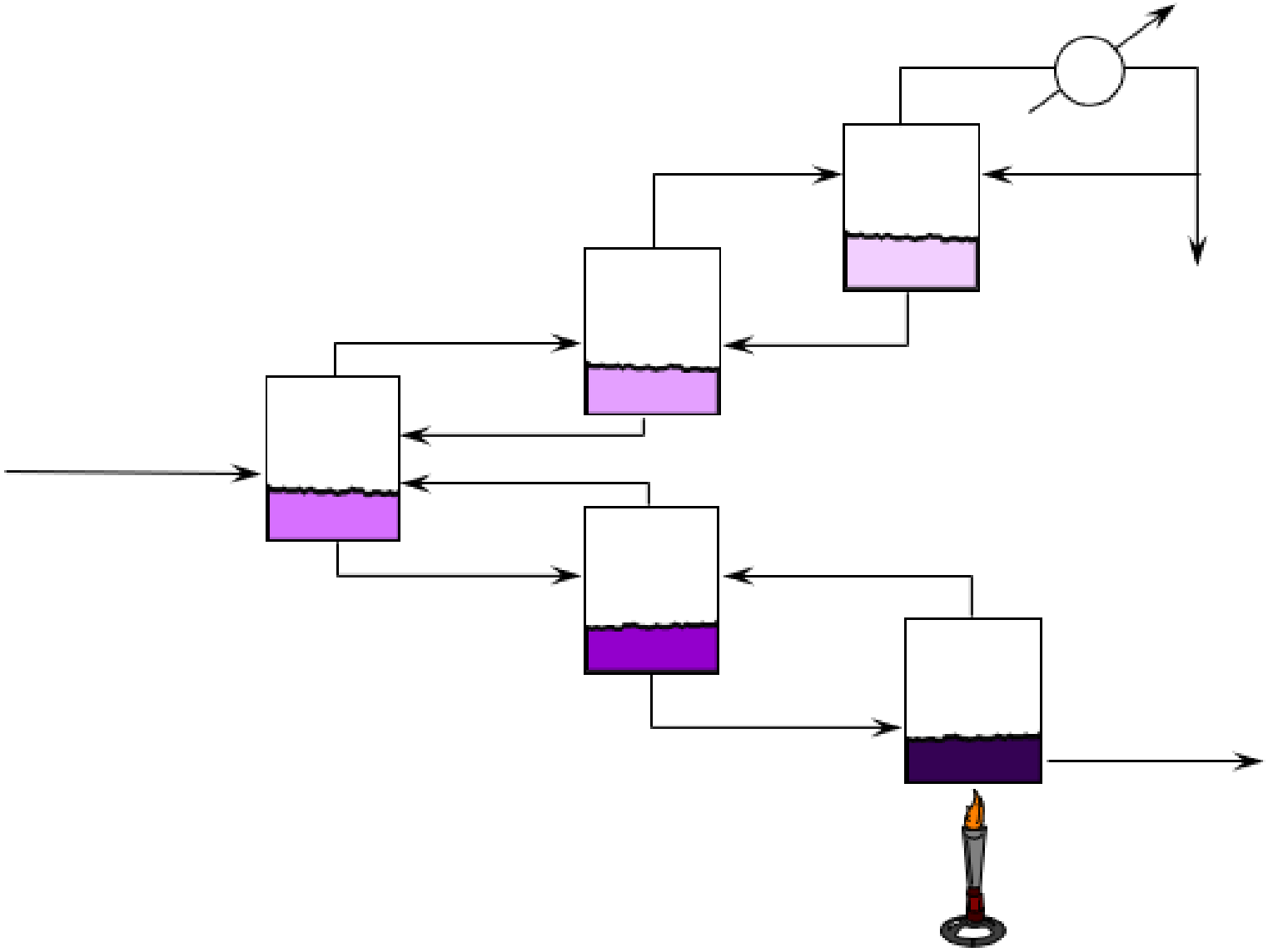
10/21/2021

Agenda

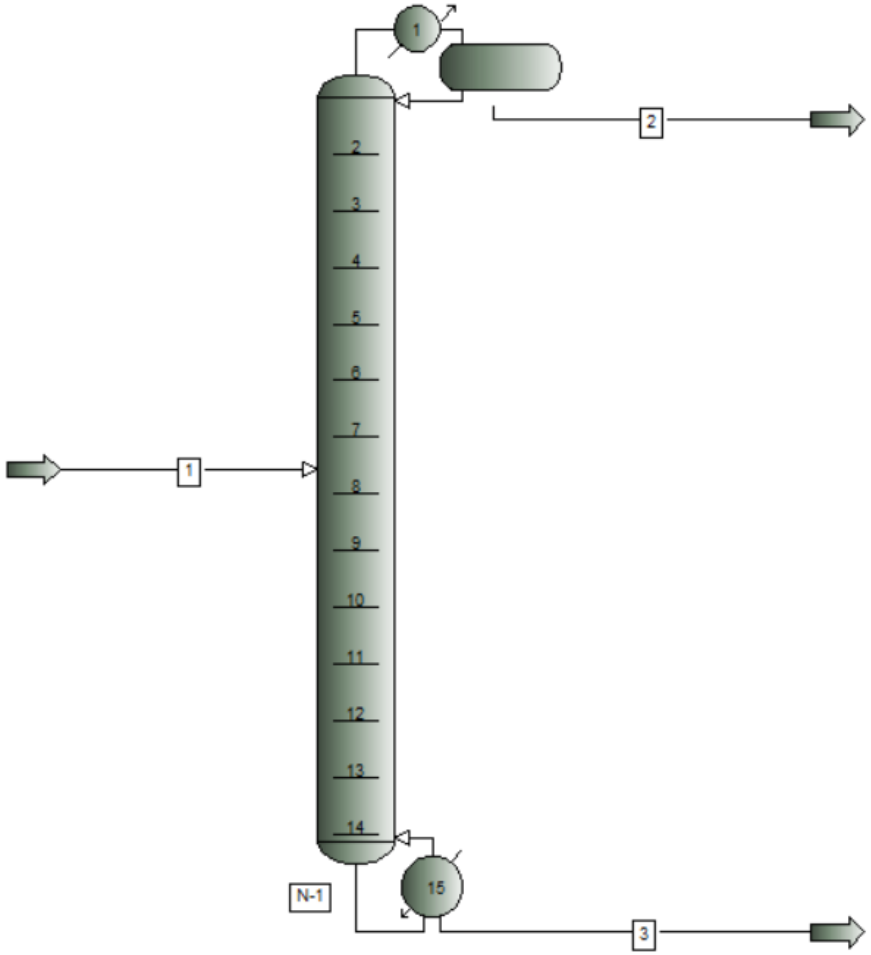
- Convergence
- Damping
- Estimates
- Initial Specifications
- Algorithms
- Errors
- Strategy

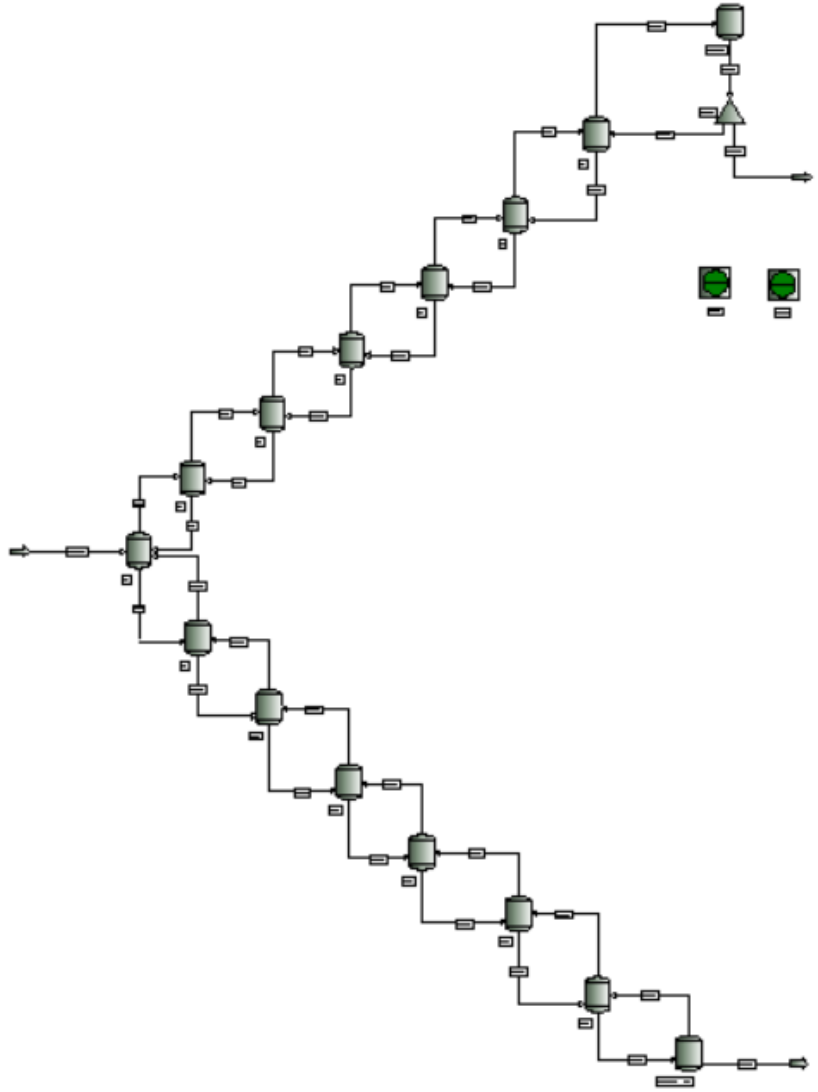


Convergence

Background

Equilibrium Stages

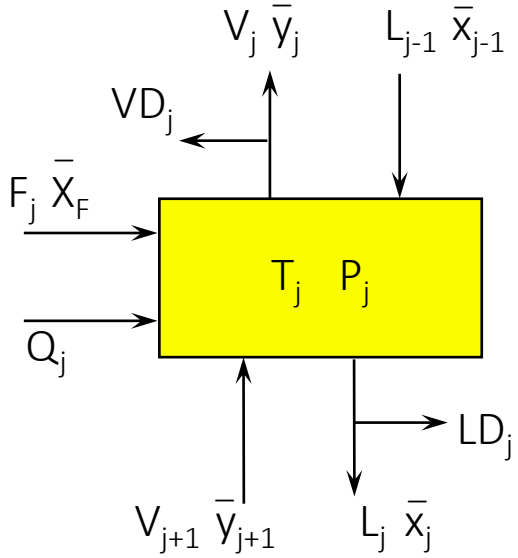




Convergence

Equations

- Mass and energy must be conserved
- The vapor and liquid leaving a stage must be in equilibrium
- The vapor and liquid mole fractions must sum to 1

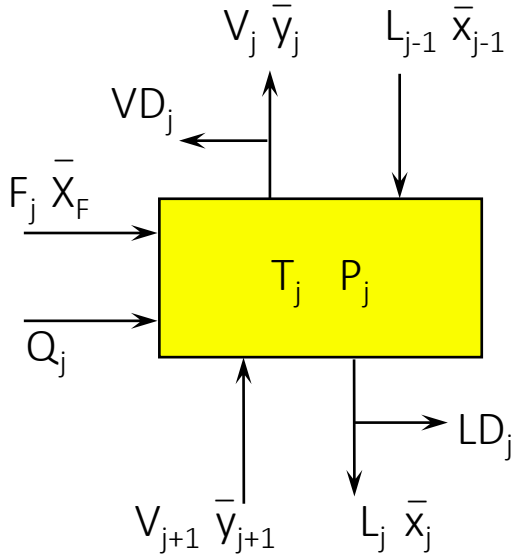


M	Mass
E	Equilibrium
S	Summation
H	Enthalpy

Convergence

Equations

- Number of equations = NT(2NC+3)
  - Example if you have 20 trays and 20 components
  - 20(40+3) = 860 equations
- Multiple non-blended petroleum assays feeding a 20-tray column
  - 10,000+ equations
- Equations are nonlinear
- All of PRO/II's distillation methods are iterative



Non-Convergence

5-Reasons

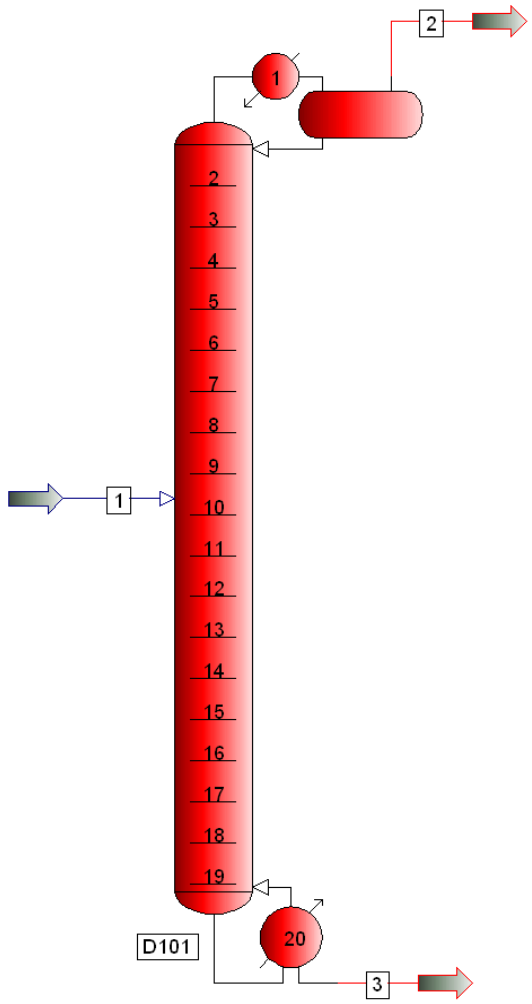
1) Improper Damping

2) Unsuitable Column Algorithm / Estimation Method

3) Initial Estimates are too far / too close to solution

4) Improper or Infeasible Specs

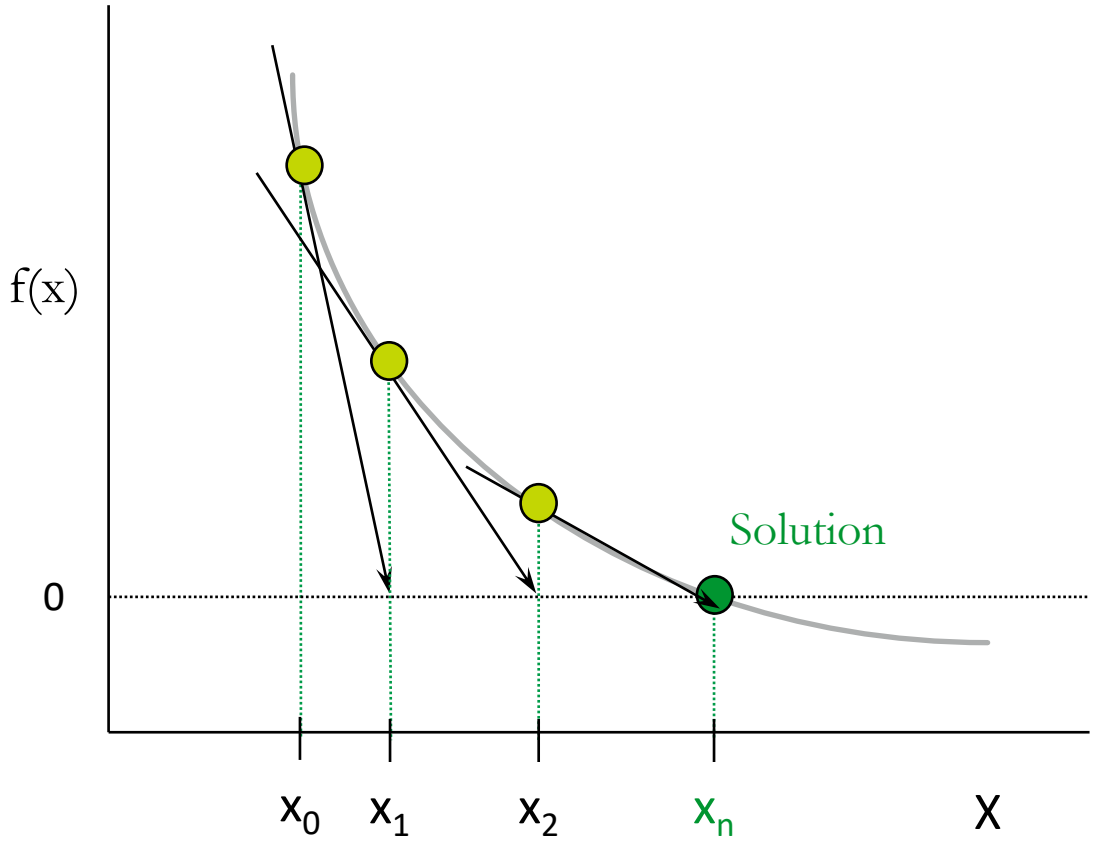
5) Not Enough Iterations



Damping

Convergence

Newton's Method



Convergence

Newton's Method

"When you throw the football, only three things can happen – and two of em ain't good"

Woody Hayes, Ohio State Football Coach 1966

The same is true for trying to converge a distillation column

1) Converge
2) Diverge
3) Oscillate

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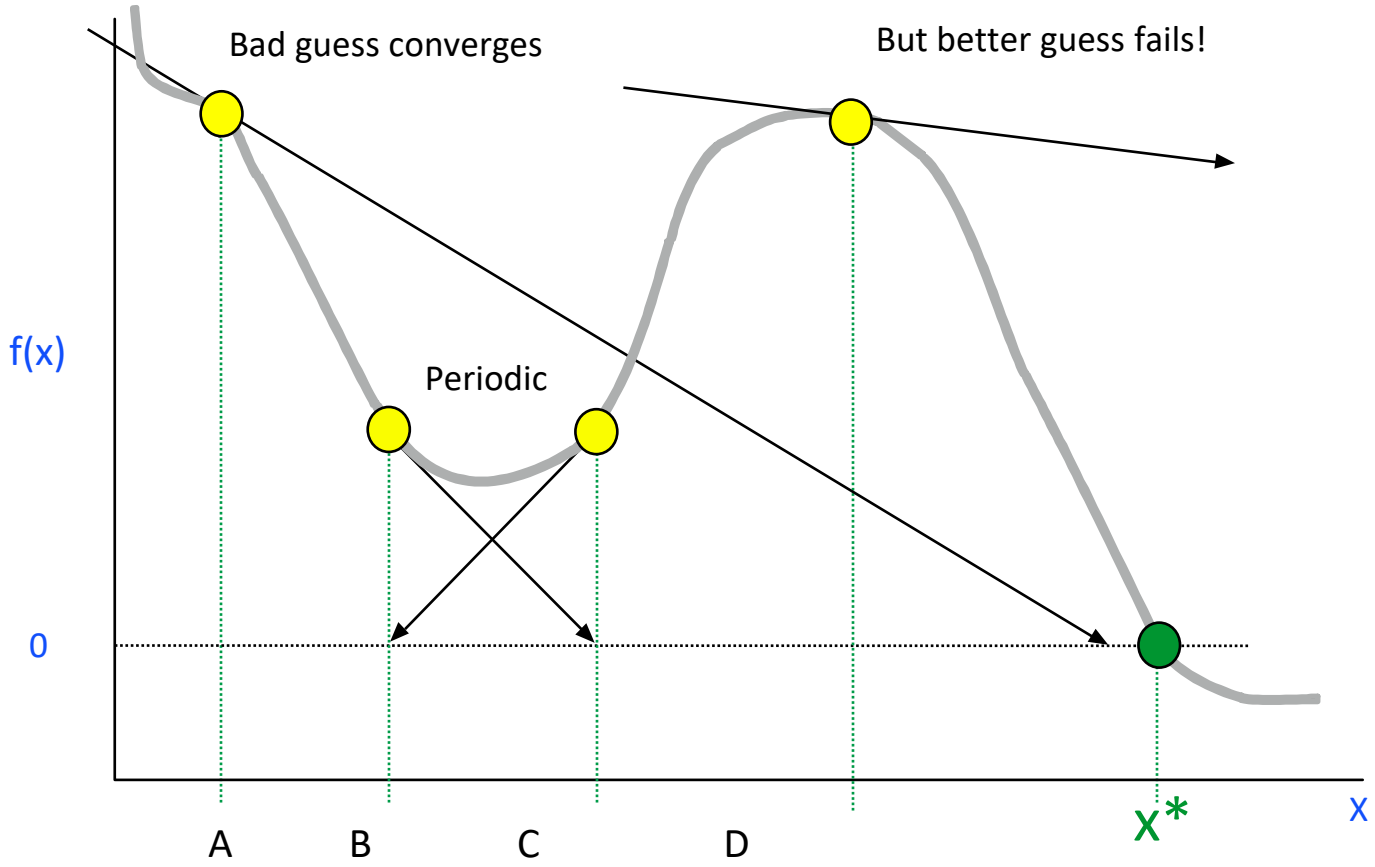
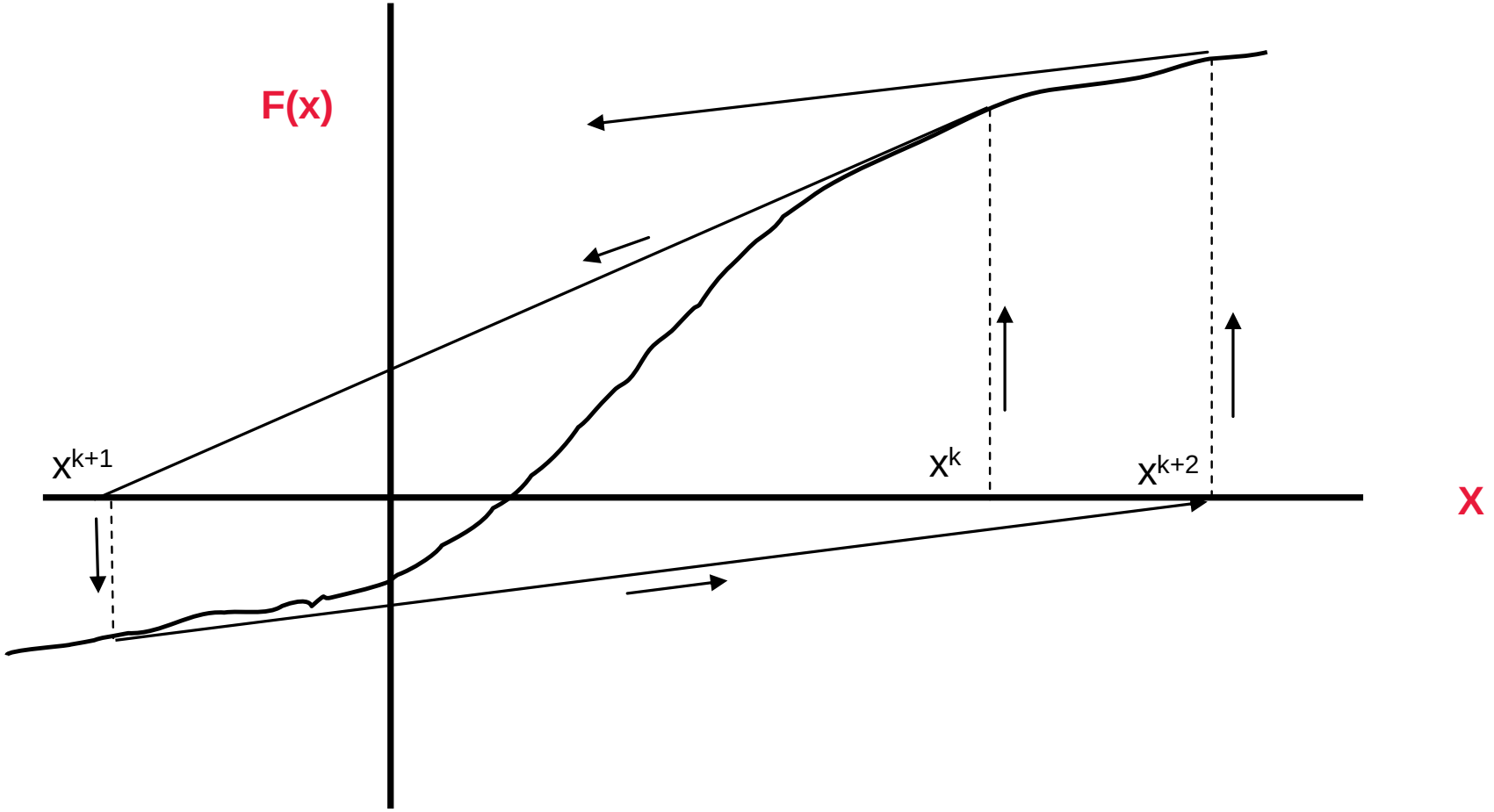
Background

Potential Issues



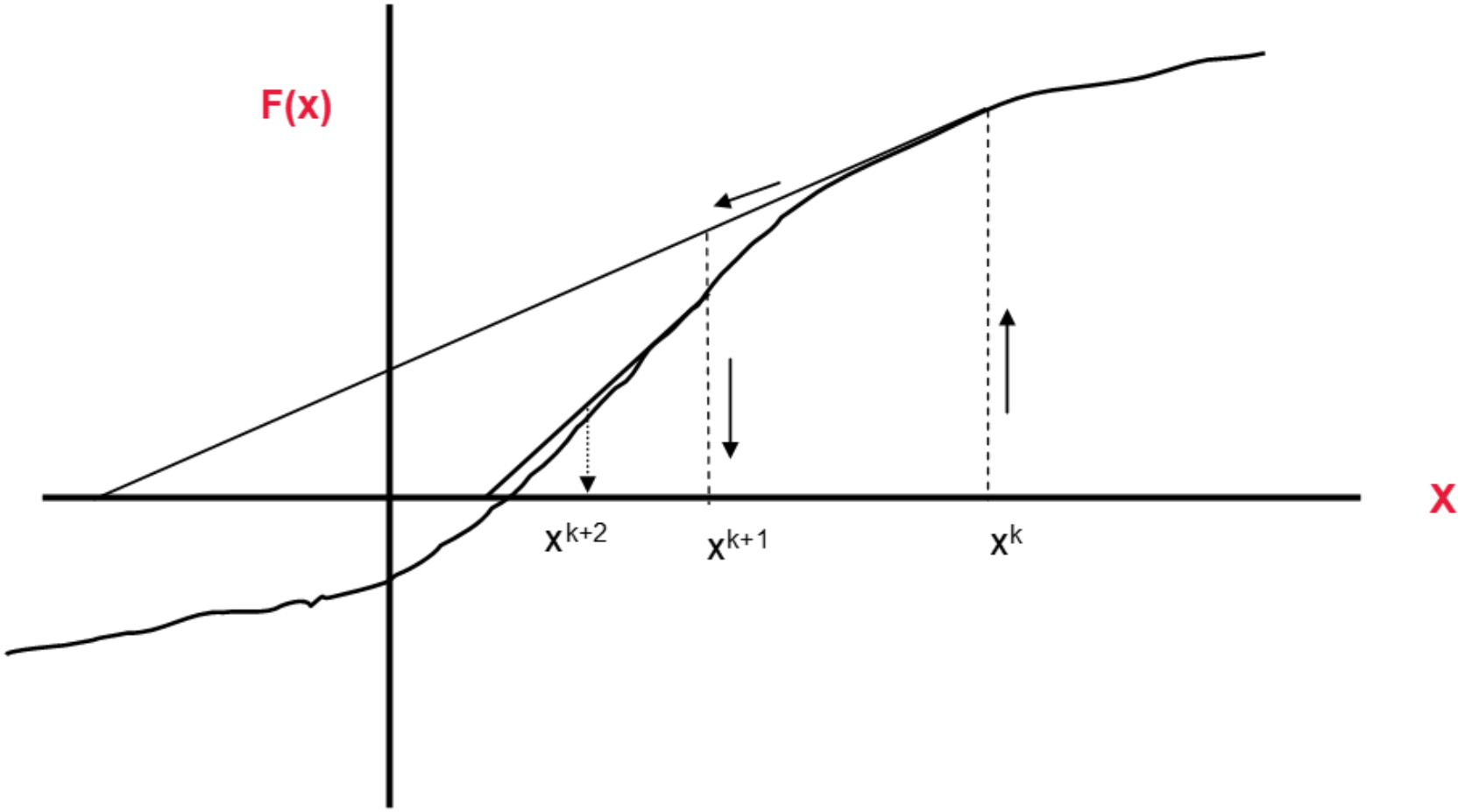
Background

Diverging Sequence



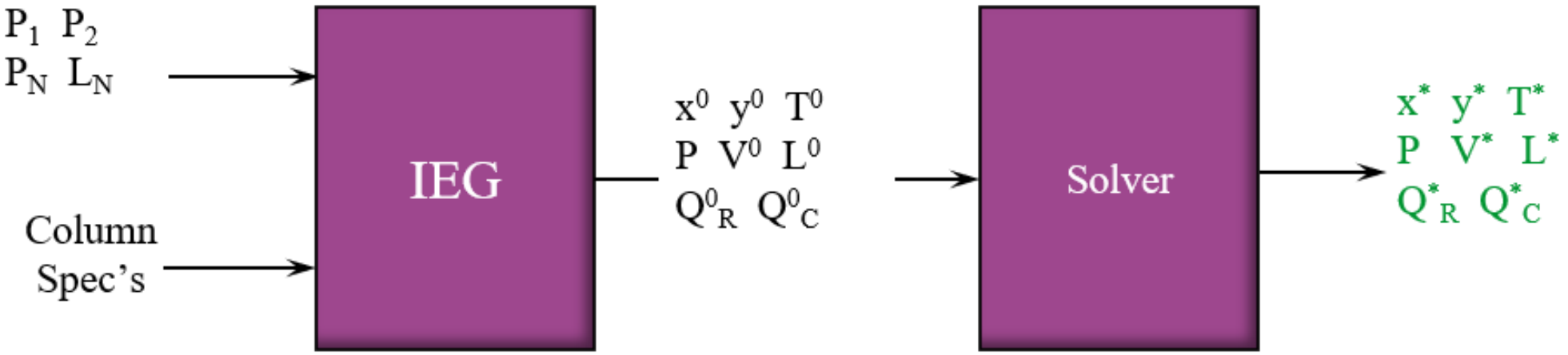
Background

Diverging Sequence



Estimates

Estimates

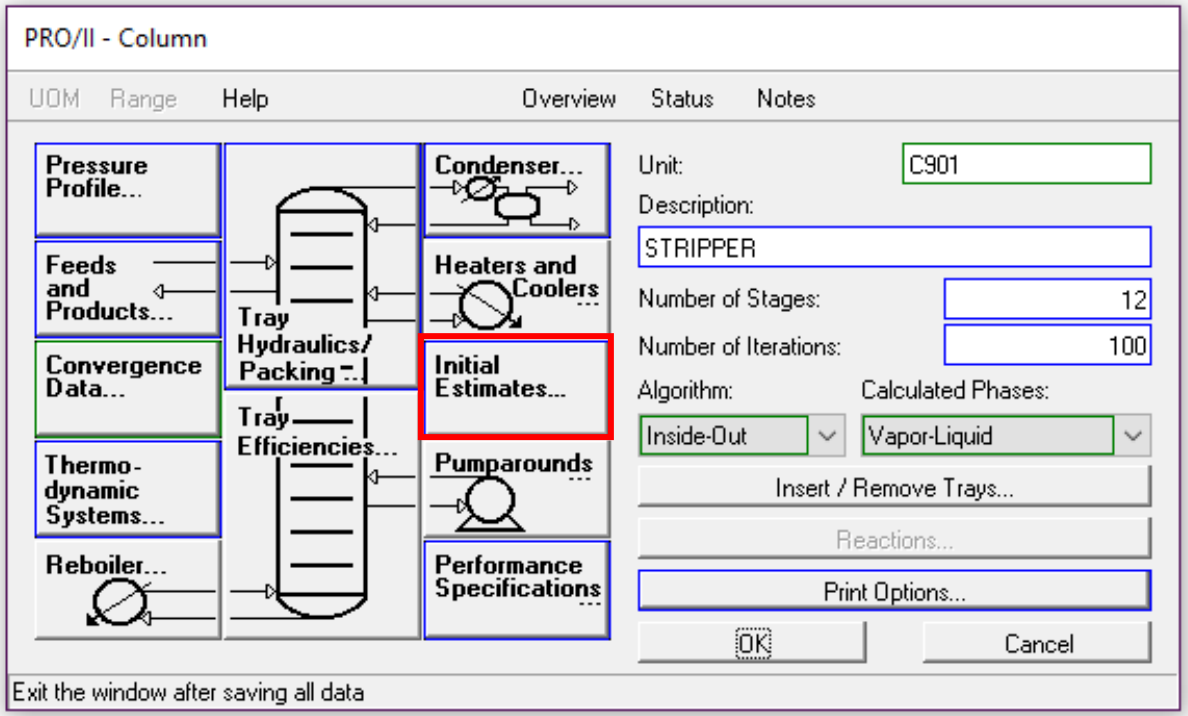


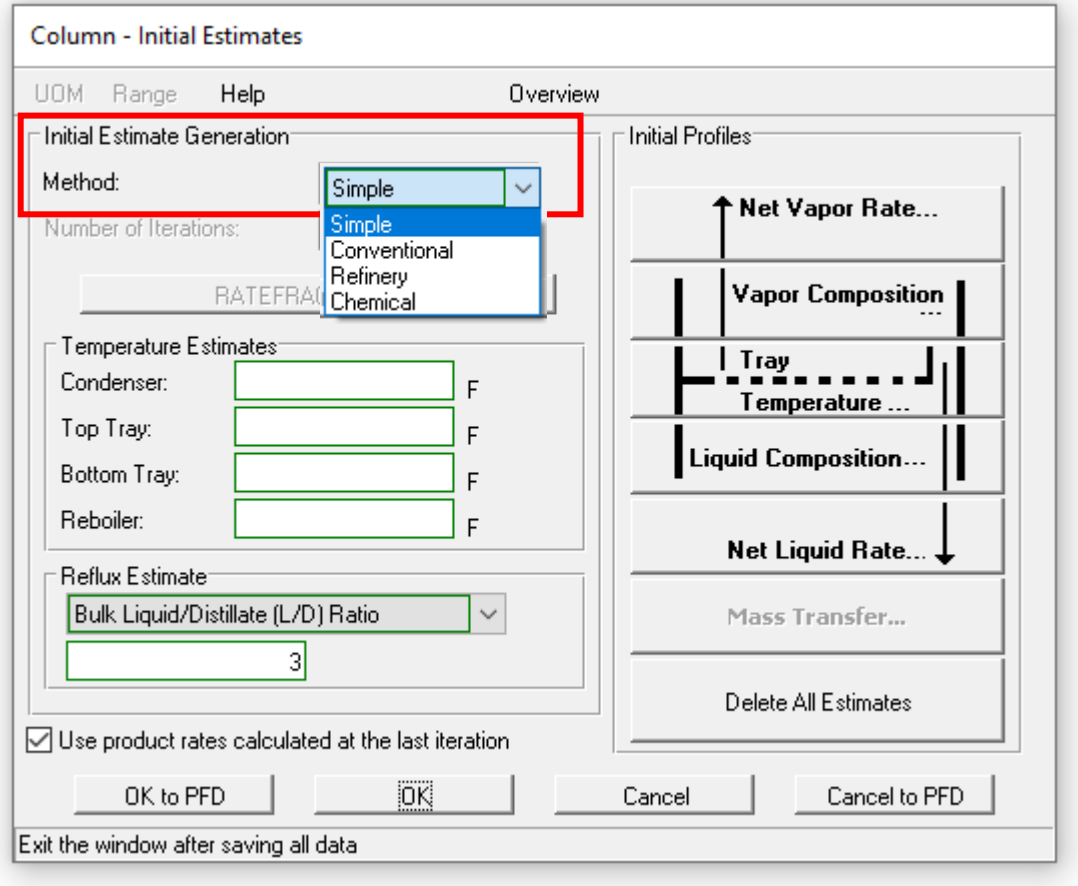
You supply column specs and guesses for a few variables...

IEG calculates initial estimates for all column variables...

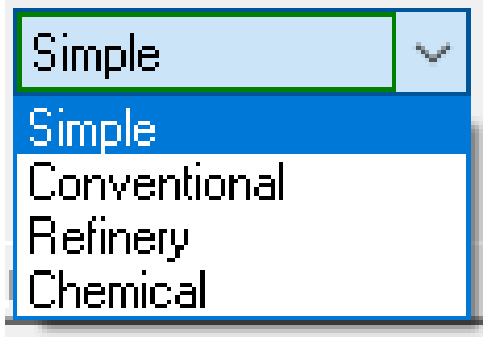
Solver (I/O, chemdist) converges on solution

Estimates





Estimates



SIMPLE

- Default for columns without a condenser or a reboiler or both
- The column profiles are determined by simple material balances.
- Temperatures are determined by estimating the product compositions.

CONVENTIONAL

- Default for columns with both a condenser and a reboiler
- Works well with most columns
- Fenske shortcut distillation calculations are used.
- Strongly dependent on your product rate estimates

REFINING

- Complex refinery columns (e.g., Crude, Vacuum, FCC main fractionator, Coker)
- A multi-product shortcut technique developed by Aveva is to generate the estimates for these columns.

CHEMICAL

- Non-ideal thermodynamics (e.g., azeotropic and extractive distillation).
- Calculates of a series of adiabatic flashes up and down the column trays several times as needed to generate a good composition starting profile.
- Slow

Initial Specifications

Specifications

Initial Column Setup

Feed Location

- Poor location can result in a compositional pinch that cannot be solved

Reflux

- Should be safely above the minimum (simulation can become unstable as the minimum reflux is approached)

Condenser and Reboiler Issues

- Bubble point condenser with non-condensables
- Fixed duty limitations
- Specifying duties and reflux

```
*** ERROR ***  The temperature of the TFIX condenser ( 110 ) is ABOVE the
               bubble point temperature of the condenser liquid ( 97.335 ).
```

Specifications

Temperature

Feed Temperature

- Convergence problems in the simulation might represent actual physical problems

Temperature and Product Spec on a Tray

- There is only a narrow range of convergence

Specifying Tray Temperatures

- Use only where composition changes significantly in the column

Specifications

Products

More Than One

- Not all methods will solve (I/O is the best)
- Replace a compositional specification with a RRatio or product rate

Two Compositional Specifications for one Product

- May be impossible
- Has a chance if the relative volatilities are high enough

Same Component Specification in Different Products

- Feasible but difficult
- Has a chance if the relative volatilities are high enough
- Difficult if the concentrations are small

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Specifications

Products (cont)

High Purity Specification

- Impurity specs are easier to hit

Compositional and Product Flow

- May clash
- Free one and specify something else

Specifying all Product Flows

- No freedom to establish a material balance
- At least one product flow rate should be allowed to float

Specifications

Products (cont)

Infinite Solutions

- Never use 0 or 100 in a specification

Unfeasible

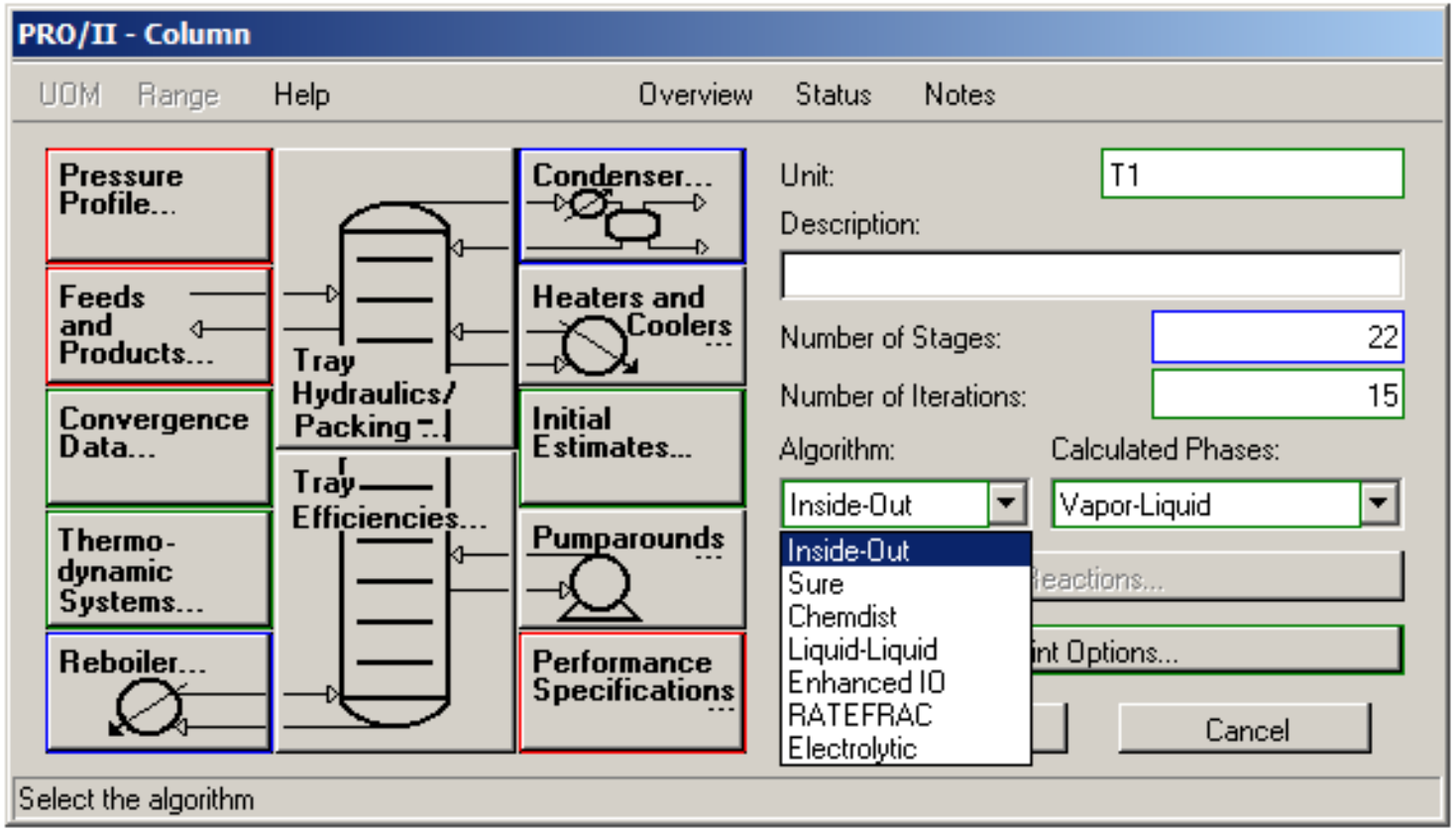
- 300 lbmol/hr propane in the OVHD – only 250 lbmol/hr feed
- Recover specifications are initially safer

Algorithms

Algorithms

Types of Distillation

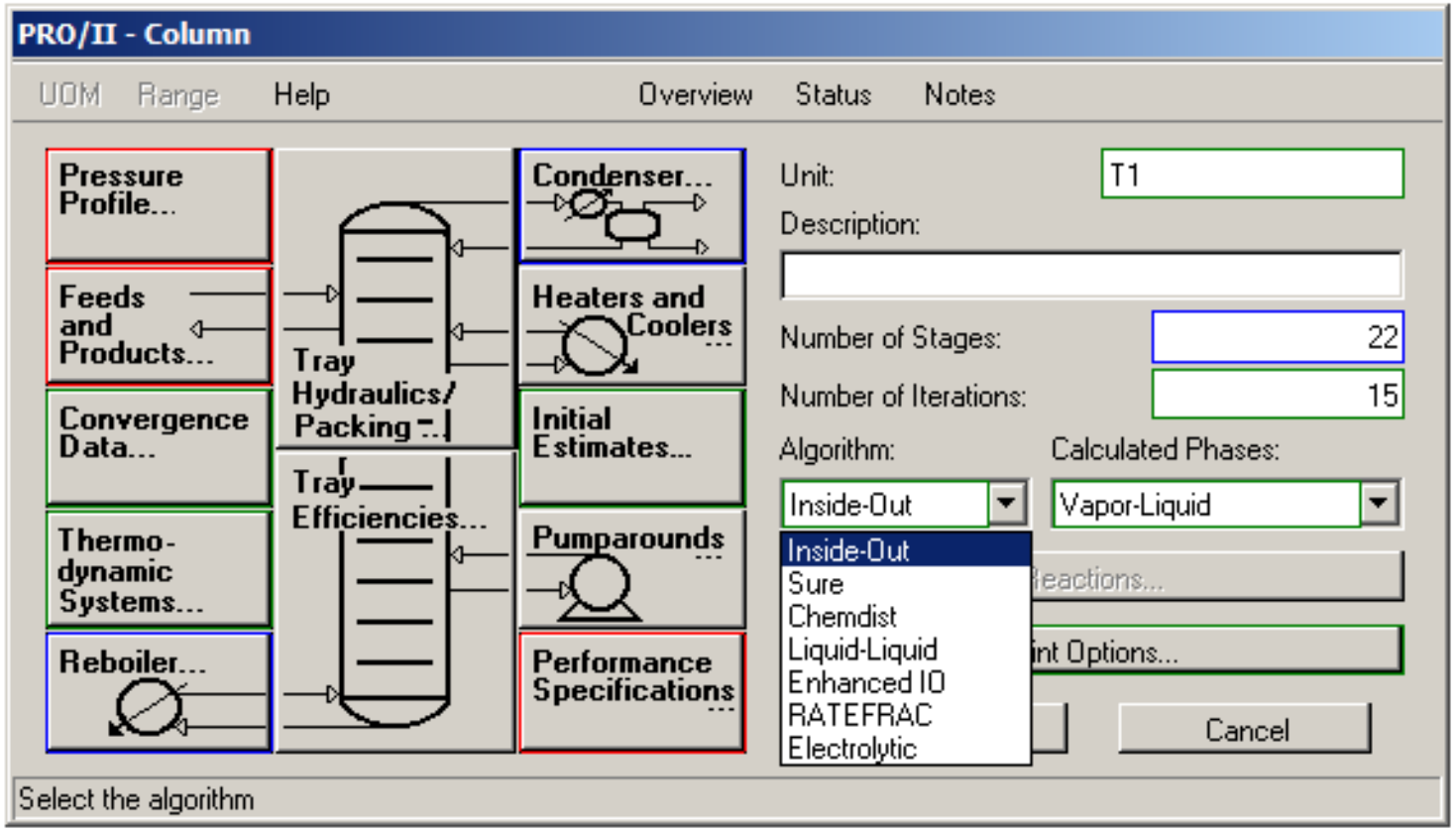
- Simple / Ideal Separation
- Wide and Narrow Boilers
- Azeotropic
- VLE / VLLE
- Electrolytic
- Reactive
- Rate Based
- Liquid-Liquid



Algorithms

Mathematical Models

- Inside-Out (I/O)
- Sure
- Chemdist
- Liquid-Liquid
- Enhanced I/O
- RATEFRAC
- Electrolytic



Algorithms

Mathematical Models

Choosing a column algorithm is based on two factors:

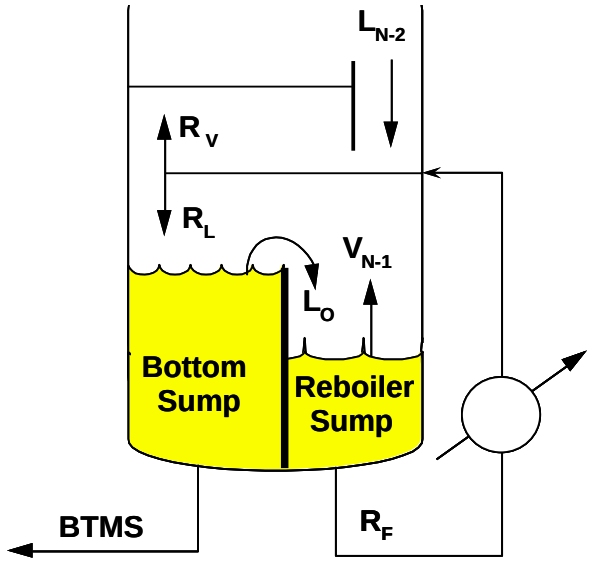
- The thermodynamic complexity of the chemical species
- The mechanical complexity of the column

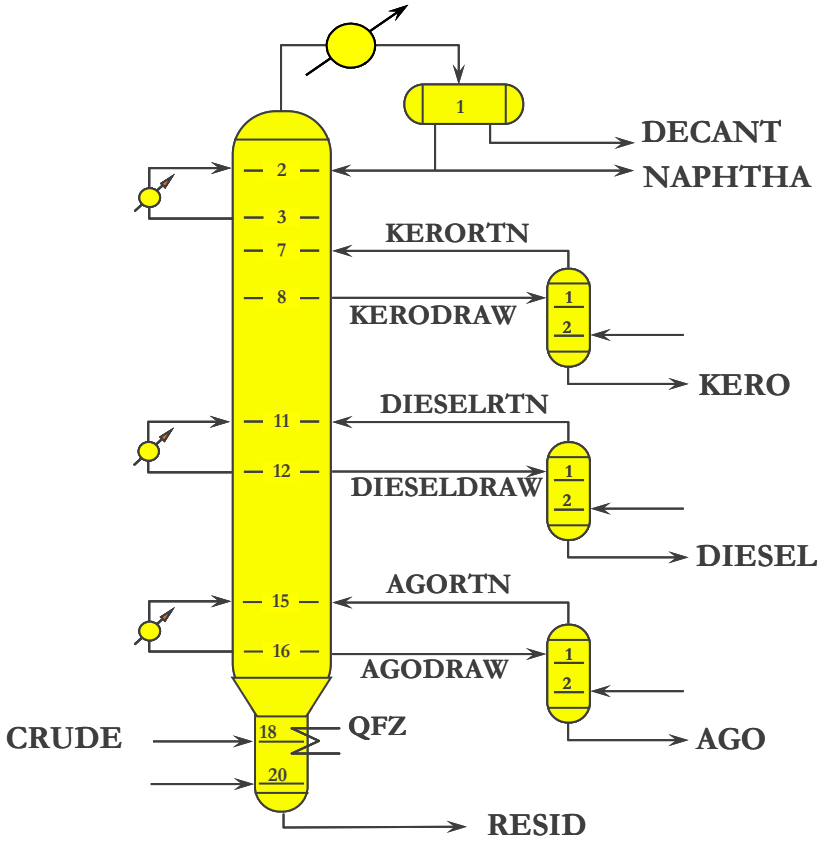
Identical results are obtained regardless of algorithm used

Algorithms

Inside-Out (I/O)

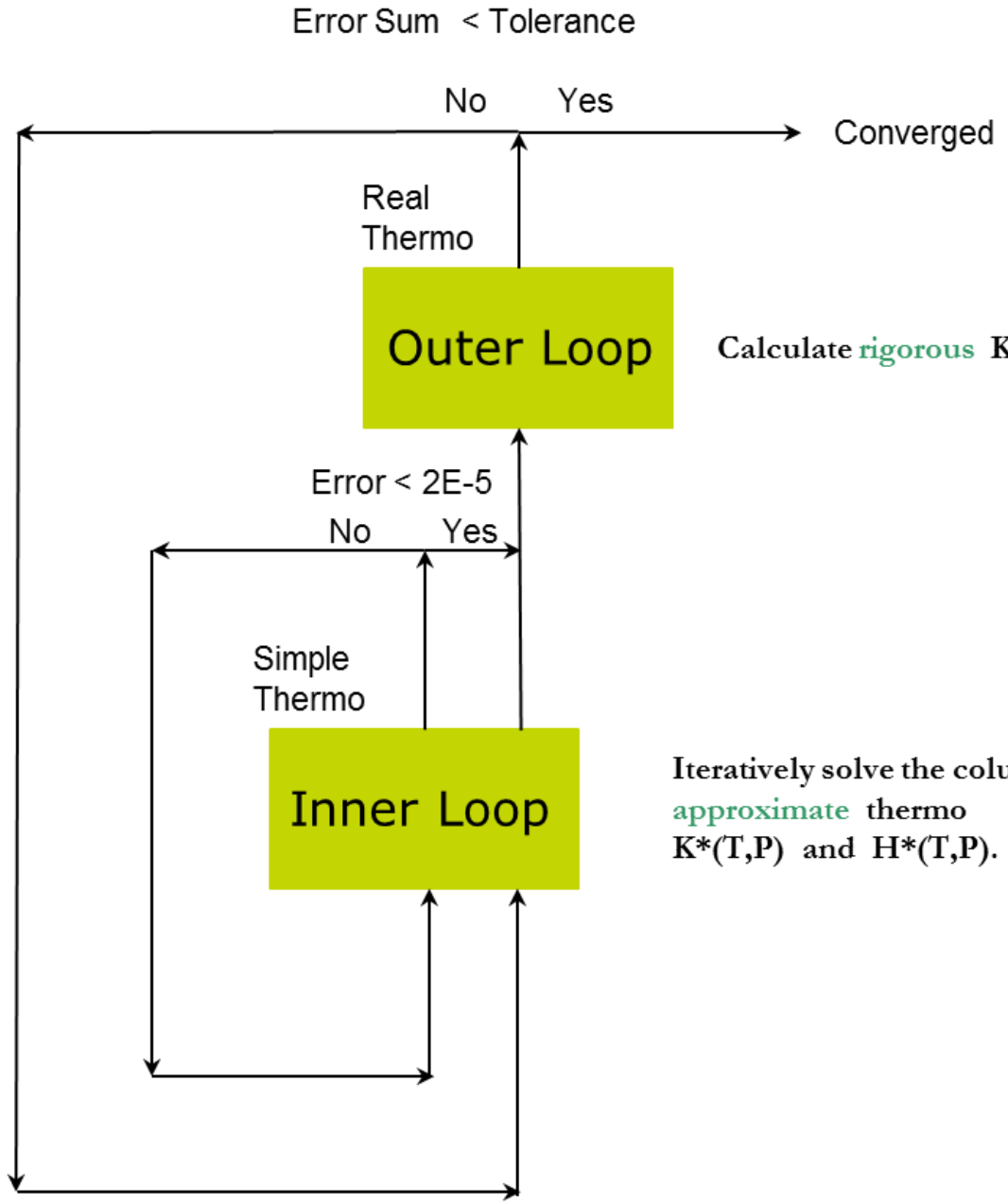
- Thermodynamically simple but mechanically complex
- Robust
- Fast
- No VLLE





Algorithms

Inside-Out (I/O)



Calculate rigorous K(x,T,P), H(x,T,P)

Iteratively solve the column equations using approximate thermo K*(T,P) and H*(T,P).

Algorithms

Inside-Out (I/O)

- To converge the inner loop the sum of the errors (Enth+Spec) < 2.0 E-05
- If the inner loop fails to converge and the (Enth+Spec) > 1, look for gross errors
- If the outer loop oscillates - the simple thermo assumption is probably not valid.

```
ITER   2 E(K) = 2.192E-01 E(ENTH+SPEC) = 8.474E-04   E(SUM) = 4.180E+00
           DAMP = 8.000E-01
         INNER  0 : E(ENTH+SPEC) = 6.146E-02
         INNER  1 : E(ENTH+SPEC) = 1.759E-02   ALPHA =  1.0000
         INNER  2 : E(ENTH+SPEC) = 9.547E-03   ALPHA =  1.0000
         INNER  3 : E(ENTH+SPEC) = 3.448E-03   ALPHA =  1.0000
         INNER  4 : E(ENTH+SPEC) = 1.724E-03   ALPHA =  1.0000
         INNER  5 : E(ENTH+SPEC) = 1.432E-03   ALPHA =  1.0000
         INNER  6 : E(ENTH+SPEC) = 7.517E-04   ALPHA =  1.0000
         INNER  7 : E(ENTH+SPEC) = 5.832E-04   ALPHA =  0.2500
         INNER  8 : E(ENTH+SPEC) = 2.658E-04   ALPHA =  1.0000
         INNER  9 : E(ENTH+SPEC) = 2.037E-04   ALPHA =  1.0000
         INNER 10 : E(ENTH+SPEC) = 1.878E-05   ALPHA =  1.0000
ITER   3 E(K) = 8.743E-02 E(ENTH+SPEC) = 1.878E-05   E(SUM) = 1.105E+00
```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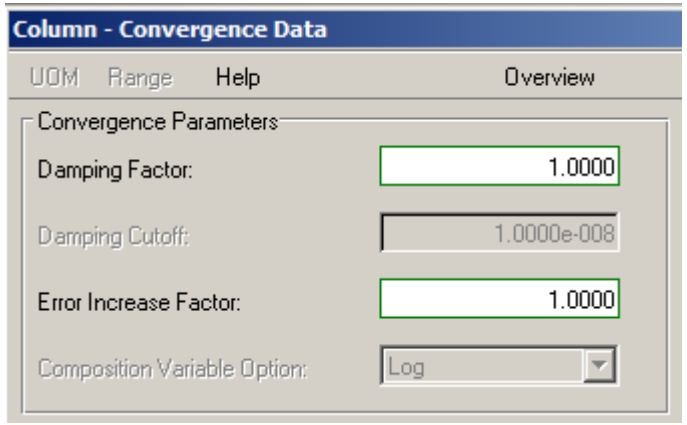
Algorithms

Oscillations




```
ITER 11 E(K) =  9.065E-02 E(ENTH+SPEC) =  2.085E-06  E(SUM) =  8.449E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  5.21674E-03
      INNER  1 : E(ENTH+SPEC) =  1.79435E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  3.20436E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  2.80296E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  3.73622E-06  ALPHA =  1.00000E+00
ITER 12 E(K) =  9.049E-02 E(ENTH+SPEC) =  3.736E-06  E(SUM) =  1.003E+00
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  5.62395E-03
      INNER  1 : E(ENTH+SPEC) =  3.07634E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.73324E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  8.44629E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  1.00291E-05  ALPHA =  1.00000E+00
ITER 13 E(K) =  1.072E-01 E(ENTH+SPEC) =  1.003E-05  E(SUM) =  9.774E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  6.00867E-03
      INNER  1 : E(ENTH+SPEC) =  1.53412E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  3.58182E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  4.32519E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  5.34562E-06  ALPHA =  1.00000E+00
ITER 14 E(K) =  9.174E-02 E(ENTH+SPEC) =  5.346E-06  E(SUM) =  1.043E+00
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  4.61421E-03
      INNER  1 : E(ENTH+SPEC) =  1.07726E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.99044E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  1.08450E-04  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  2.16836E-05  ALPHA =  1.00000E+00
      INNER  5 : E(ENTH+SPEC) =  1.41765E-06  ALPHA =  1.00000E+00
ITER 15 E(K) =  8.358E-02 E(ENTH+SPEC) =  1.418E-06  E(SUM) =  7.879E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  4.58525E-03
      INNER  1 : E(ENTH+SPEC) =  2.89594E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.48525E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  2.84930E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  2.14820E-06  ALPHA =  1.00000E+00
```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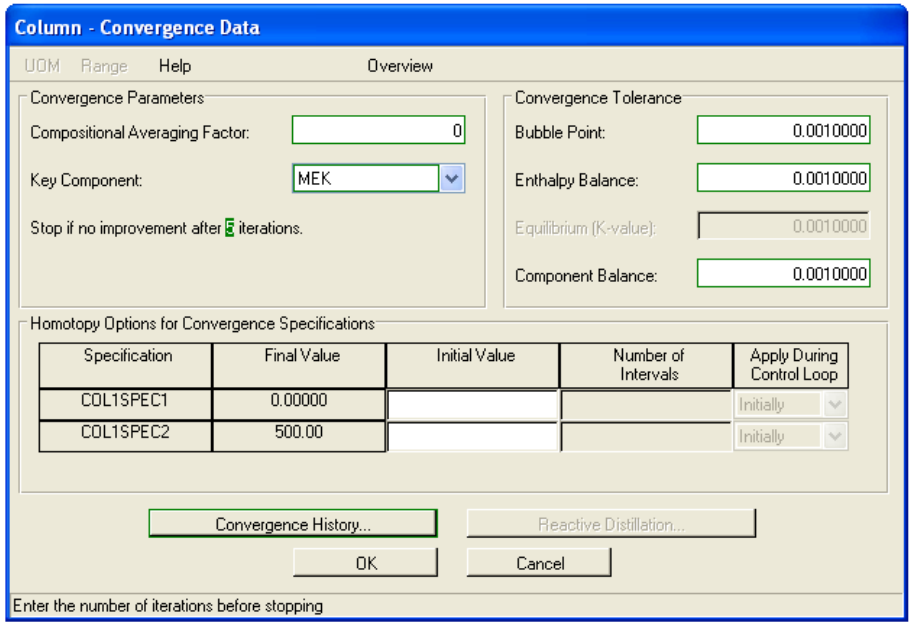
Algorithms

Sure Method

- This method uses a modified Newton-Raphson solution technique with equation partitioning (proprietary equation tearing)
- Side columns are solved as recycles
- Somewhat sensitive to initial estimates
- PA's allowed
- Thermosiphons (as of 9.0)
- VLLE



Algorithms

Sure Method

SURE ITER	ALFA	ALFA MAX	ERROR(H)	ERROR(E)	ERROR(M)	ERROR SUM
1	3.921E-04	3.921E-04	-5.528E+01	-9.833E+01	1.331E+03	6.226E+02
2	3.351E-01	3.351E-01	-4.738E+01	-4.553E+01	7.389E+02	2.685E+02
3	8.372E-01	8.372E-01	6.111E+01	-2.051E+01	5.176E+02	2.333E+02
4	2.659E-01	2.659E-01	7.002E+01	-2.291E+01	3.989E+02	1.843E+02
5	5.428E-01	5.428E-01	4.772E+01	-1.441E+01	4.313E+02	1.078E+02
6	9.328E-01	9.328E-01	2.487E+01	-7.047E+00	4.902E+02	5.284E+01
7	1.000E+00	1.000E+00	1.159E+01	-3.284E+00	3.121E+02	2.533E+01
8	1.000E+00	1.000E+00	4.924E+00	-1.552E+00	1.936E+02	1.209E+01
9	1.000E+00	1.000E+00	2.083E+00	-6.549E-01	1.451E+02	5.009E+01
10	1.000E+00	1.000E+00	8.183E-01	-2.712E-01	1.289E+02	1.978E+00
11	1.000E+00	1.000E+00	3.423E-01	-1.035E-01	1.266E+02	1.045E+00
12	4.225E-01	1.000E+00	-8.785E-02	-1.698E-01	1.168E+02	9.410E-01
13	2.746E-01	1.000E+00	9.172E-02	-2.650E-01	2.443E+00	1.611E+00
14	1.000E+00	1.000E+00	2.364E-02	2.407E-02	1.205E+00	2.377E-01
15	1.000E+00	1.000E+00	1.342E-02	2.425E-02	-5.812E-01	1.681E-01
16	1.000E+00	1.000E+00	4.062E-03	-9.632E-03	-3.715E-01	7.621E-02
17	6.500E-01	1.000E+00	1.254E-03	-2.133E-03	-1.265E-01	1.501E-02
18	2.746E-01	1.000E+00	-3.587E-03	1.009E-02	-9.593E-04	5.330E-02
19	1.000E+00	1.000E+00	-1.662E-03	-5.291E-03	-8.748E-03	2.997E-02
20	1.000E+00	1.000E+00	-7.381E-04	1.715E-03	-1.847E-04	8.595E-03
21	1.000E+00	1.000E+00	-2.685E-04	4.508E-04	-5.100E-05	2.433E-03

UNIT 2 SOLVED

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Algorithms

Sure Method

Advantages

- Two liquid phases may be considered
- A free water phase and water draws are permitted in columns at trays below the condenser
- Total pumparounds are permitted
- Handles non-ideal interactions

Disadvantages

- Slow
- Need accurate estimates
- Side columns are handled as recycle streams

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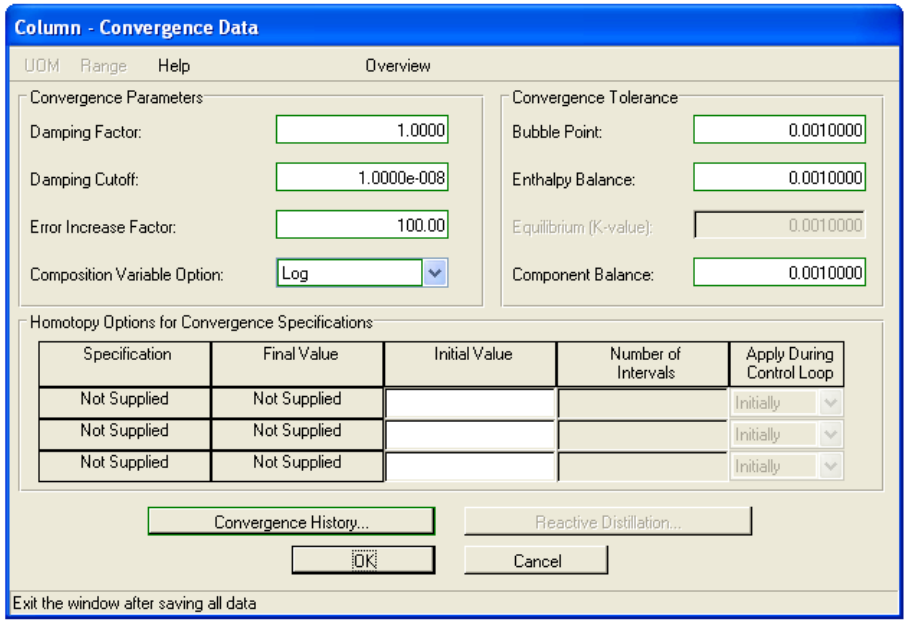
Algorithms

Chemdist

- Mechanically simple – thermodynamically complex
- It uses a modified Newton Raphson algorithm with a proprietary matrix solver developed by SimSci.
- PRO/II checks the VLE trays for possible VLLE behavior. If VLLE behavior is detected, the column may be resolved using VLLE system for these trays.
- No thermosiphons
- No PA’s
- Very sensitive to initial estimates
- Reactive distillation
- Azeotropic distillation



Algorithms

Chemdist

```
** WARNING **  UNIT 1, 'W-10', 'DEHYD COL' - TWO LIQUID PHASES have been
               detected on the following stages that were declared with VLE
               thermodynamic METHOD sets:
          TRAY    L1 FRACTION
          ----    -----------
             5      0.2012
** WARNING **  Tray 5 has been CHANGED to VLLE thermodynamic METHOD set 2 to

                    ======== Scaled & Normalized SQRT(SUM(ERR**2)) =======
                     Component     Component       Stage        Average    VLLE
      Iter  Alpha       VLE         M-Balance     H-Balance     SumX+SumY   Range
      ---- ------  ------------  ------------  ------------  ------------ -----
        1  1.0000   3.007E-03     1.226E-05 *   3.152E-04     2.643E-18    1- 5
        2  1.0000   7.186E-04     1.835E-06 *   3.774E-05     5.287E-18    1- 5
        3  1.0000   2.273E-04     1.107E-06 *   2.119E-05     8.554E-18    1- 5
        4  1.0000   7.215E-05     6.053E-07 *   4.986E-06 *   5.287E-18    1- 5
             Overall Material Balance Not Satisfied for Component (  2) H2O
        5  1.0000   1.248E-05 *   3.043E-07 *   1.168E-06 *   5.911E-18    1- 5
        6  1.0000   4.877E-06 *   1.525E-07 *   4.275E-07 *   5.911E-18    1- 5
      -----------  ------------  ------------  ------------  ------------
      Max - Error   2.198E-04 *   9.599E-06 *   6.099E-06 *   2.220E-16
          - Tray    --   3  --     --   2  --     --   6  --
          - Comp.     TOLUENE         H2O

       * - Maximum error satisfies convergence tolerance.

     UNIT     1     SOLVED
*** PROBLEM SOLUTION REACHED
*** Run completed - Case solved
```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Convergence Errors

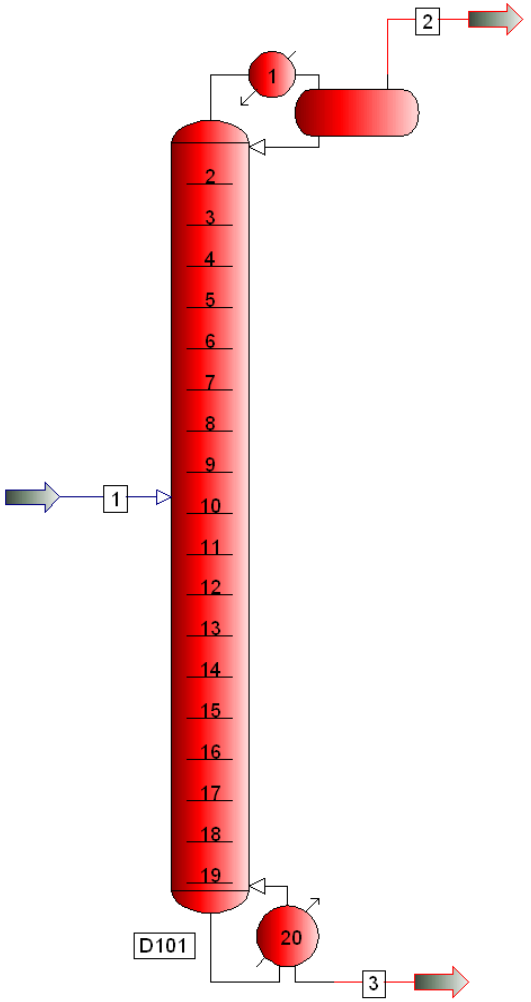
Convergence Errors

Check the Column Profile and Iterations Messages

COLUMN SUMMARY

TRAY	TEMP DEG F	PRESSURE PSIA	NET FLOW RATES LIQUID	VAPOR	FEED LB-MOL/HR	PRODUCT
1	194.7	20.80	3237.1		1919.9M	700.5V
2	279.2	20.96	11864.5	2201.9		
3	130.1	21.11	53462.4	10829.3		
4	-16.5	21.27	2473.9	52427.1		
5	-23.5	21.42	9.90E+06	1438.7		
6	-423.7	21.58	1939.7	9.90E+06		
7	199.2	21.73	1035.7	904.5		
8	205.4	21.89	1035.4	0.5		
9	185.5	22.04	1035.5	0.2		
10	170.2	22.20	1035.7	0.3		
11	163.9	22.35	1035.9	0.5		
12	166.4	22.51	1036.1	0.7		
13	177.8	22.66	1036.5	0.9		
14	198.3	22.82	1037.6	1.3		
15	224.7	22.97		2.4	70.2V	1289.6L

```
*** PROBLEM SOLUTION BEGINS
    FEED FLASH    BEGINS
    FEED FLASH    COMPLETE
    UNIT    2     BEGINS    - 'SWS1        '
            INNER  0 : E(ENTH+SPEC) = 3.493E-01
            CALCULATING NEW MATRIX
            INNER  1 : E(ENTH+SPEC) = 3.411E-01  ALPHA =  0.0113
            INNER  2 : E(ENTH+SPEC) = 3.395E-01  ALPHA =  0.0143
            INNER  3 : E(ENTH+SPEC) = 3.028E-01  ALPHA =  0.2412
            INNER  4 : E(ENTH+SPEC) = 1.669E-01  ALPHA =  0.1055
            INNER  5 : E(ENTH+SPEC) = 1.122E-01  ALPHA =  0.0391
            INNER  6 : E(ENTH+SPEC) = 1.107E-01  ALPHA = -0.0345
            INNER  7 : E(ENTH+SPEC) = 1.082E-01  ALPHA = -0.1154
            INNER  8 : E(ENTH+SPEC) = 1.026E-01  ALPHA = -0.0525
            INNER  9 : E(ENTH+SPEC) = 9.020E-02  ALPHA =  0.4426
            INNER 10 : E(ENTH+SPEC) = 5.795E-02  ALPHA =  0.3405
       ITER  1 E(K) = 7.290E+02 E(ENTH+SPEC) = 5.795E-02  E(SUM) = 9.452E+03
              DAMP = 4.000E-01
*** A FATAL ERROR OCCURRED ON ITERATION    2
*** ERROR HISTORY IS NOT AVAILABLE FOR THIS ITERATION
*** ERROR ***  UNIT 2, 'SWS1' - TEMPERATURE EXCEEDS LIMIT on tray 6.
    UNIT    2 NOT SOLVED
*** PROBLEM SOLUTION NOT REACHED
```



Convergence Errors

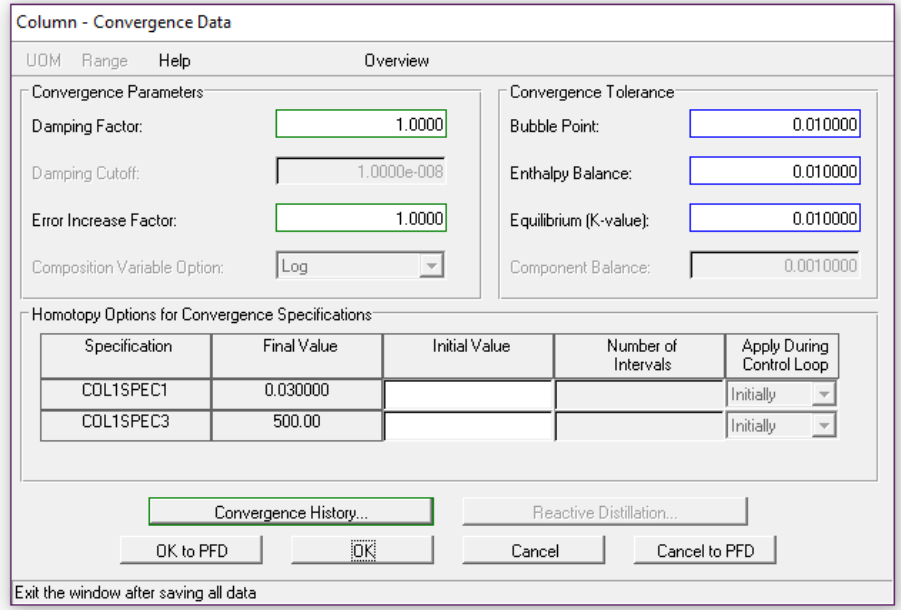
Check the Column Profile and Iterations Messages

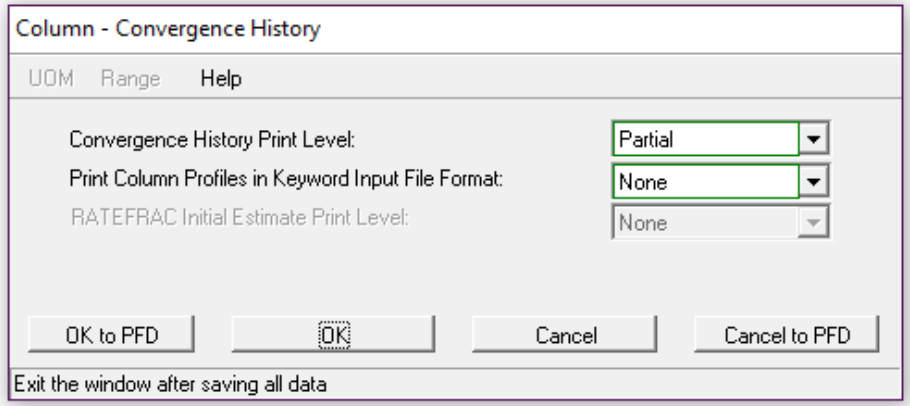
Partial - Default

```
ITER   4 E(K) = 2.969E-03 E(ENTH+SPEC) = 7.095E-06  E(SUM) = 1.442E-02
         DAMP = 1.000E+00
       INNER   0 : E(ENTH+SPEC) = 1.836E-04
       INNER   1 : E(ENTH+SPEC) = 4.197E-05  ALPHA =  1.0000
       INNER   2 : E(ENTH+SPEC) = 2.040E-06  ALPHA =  1.0000
ITER   5 E(K) = 6.939E-04 E(ENTH+SPEC) = 2.040E-06  E(SUM) = 2.260E-03
```

All

```
ITER   4 E(K) = 2.969E-03 E(ENTH+SPEC) = 7.095E-06  E(SUM) = 1.442E-02
  COMPONENT ERROR: AVG = 1.135E-04 MAX(T   4      ) = -1.231E-03
  ENTHALPY  ERROR: AVG = 6.871E-05 MAX(T 11, VAP ) = -2.287E-04
  K-VALUE   ERROR: AVG = 2.969E-03 MAX(T 10, C 10) =  1.049E-02
         DAMP = 1.000E+00
       INNER   0 : E(ENTH+SPEC) = 1.836E-04
         SPEC ERROR : AVG = 9.484E-04 MAX(SPEC   1   ) =  1.670E-03
         HBAL ERROR : AVG = 4.133E-05 MAX(TRAY   8   ) = -1.122E-04
         TEMP CHANGE: AVG = 7.998E-02 MAX(TRAY   6   ) =  2.368E-01
       INNER   1 : E(ENTH+SPEC) = 4.197E-05  ALPHA =  1.0000
         SPEC ERROR : AVG = 2.495E-04 MAX(SPEC   1   ) =  6.293E-04
         HBAL ERROR : AVG = 4.552E-06 MAX(TRAY   4   ) =  2.230E-05
         TEMP CHANGE: AVG = 7.130E-02 MAX(TRAY   5   ) = -2.721E-01
       INNER   2 : E(ENTH+SPEC) = 2.040E-06  ALPHA =  1.0000
         SPEC ERROR : AVG = 9.952E-06 MAX(SPEC   1   ) = -1.927E-05
         HBAL ERROR : AVG = 5.467E-07 MAX(TRAY   4   ) =  2.365E-06
         TEMP CHANGE: AVG = 1.541E-02 MAX(TRAY   5   ) =  3.447E-02
ITER   5 E(K) = 6.939E-04 E(ENTH+SPEC) = 2.040E-06  E(SUM) = 2.260E-03
  COMPONENT ERROR: AVG = 2.870E-05 MAX(T   4      ) = -2.055E-04
  ENTHALPY  ERROR: AVG = 1.331E-05 MAX(T 10, VAP ) = -3.883E-05
  K-VALUE   ERROR: AVG = 6.939E-04 MAX(T   7, C 10) =  1.678E-03
```





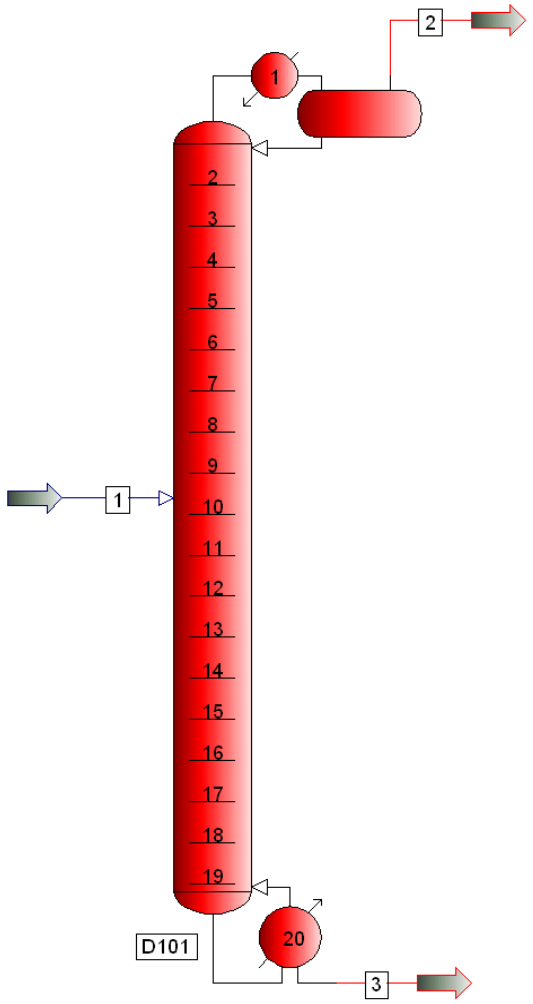
Convergence Errors

- Unsuitable Column Algorithm
- Initial Estimates are too far / too close to solution
- Improper or Infeasible Specs

```
*** ERROR ***  UNIT 1, 'D101', 'DEETHANIZER' - SINGULAR MATRIX. Please check
               input data for consistency.

*** ERROR ***  COLUMN calculations TERMINATED. The convergence error cannot be
               reduced using the newly calculated matrix.

*** ERROR ***  COLUMN calculations TERMINATED. Alpha ( the damping factor )
               was BELOW .01 for 4 consecutive iterations after 15 new matrix
               calculations.
```



Convergence Errors

Not Enough Iterations

Iterations

- Especially if damping applied
- Check the printout

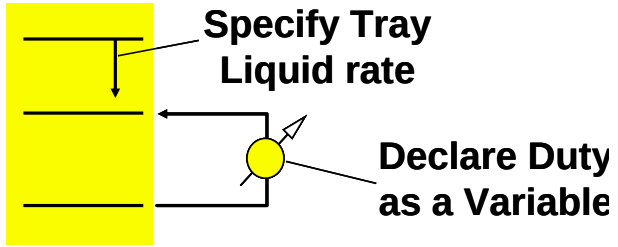
Bad Actor Components

- Water can seriously upset a VLE method
- Insure that water is not condensing on any trays in your column

```
** WARNING **  UNIT 6 - WATER SUPERSATURATION DETECTED on 1 trays. Column
                solution is likely to be erroneous. Rerun using the SURE column
                with the FREEWATER (DECANT) option enabled.
```

PA's can be Problematic

- Fix rate and duty - calculate return temperature.
- Excess cooling cause drying above PA return
- Remedy: Specify liquid flow above return tray and calculate pumparound duty



Convergence Errors

Systems with Highly Non-Ideal Thermodynamics

- You need very good estimates
- Solve with a simple approximation and then use this for a new estimate

Evaluate the Column solution

- What does the temperature/ vapor and liquid flows look like
- What specifications have and have not been met

If the Column is in a Recycle Loop

- Ensure that the vapor and liquid traffic have been established
- Ensure that the recycle loop is at a lower tolerance than the units in the loop

H2

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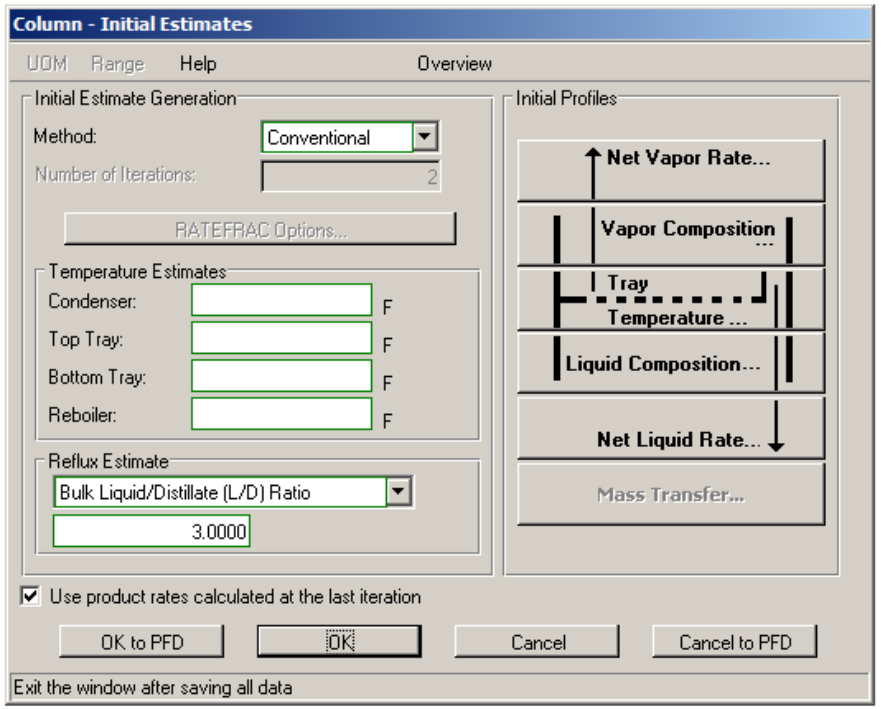
Convergence Errors

Understand how Subsequent runs are Handled in AVEVA PRO/II Simulation

- PRO/II ‘remembers’ product flow rates from previous solutions, and uses those to restart the IEG
- If the previous run did not converge, product flow rates may be very bad, and throw off the IEG for subsequent runs
- Click on ‘Restore Input Data’ in the Input menu item

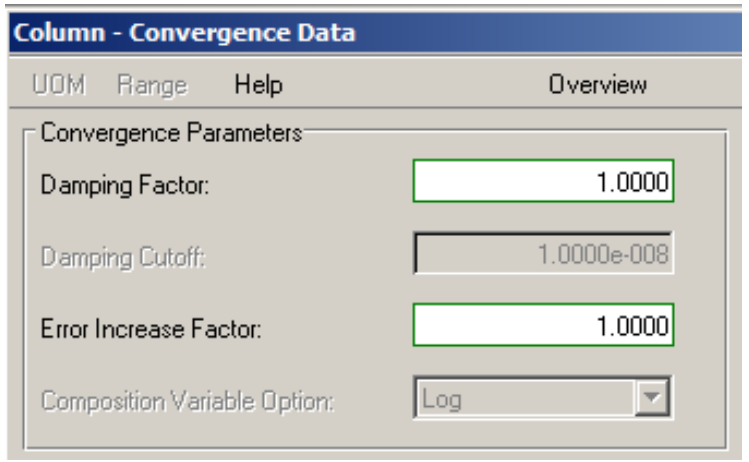


Convergence Errors

Damping

- Check the messages for a read back on how the algorithm performed

```
ITER 11 E(K) =  9.065E-02 E(ENTH+SPEC) =  2.085E-06  E(SUM) =  8.449E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  5.21674E-03
      INNER  1 : E(ENTH+SPEC) =  1.79435E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  3.20436E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  2.80296E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  3.73622E-06  ALPHA =  1.00000E+00
ITER 12 E(K) =  9.049E-02 E(ENTH+SPEC) =  3.736E-06  E(SUM) =  1.003E+00
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  5.62395E-03
      INNER  1 : E(ENTH+SPEC) =  3.07634E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.73324E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  8.44629E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  1.00291E-05  ALPHA =  1.00000E+00
ITER 13 E(K) =  1.072E-01 E(ENTH+SPEC) =  1.003E-05  E(SUM) =  9.774E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  6.00867E-03
      INNER  1 : E(ENTH+SPEC) =  1.53412E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  3.58182E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  4.32519E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  5.34562E-06  ALPHA =  1.00000E+00
ITER 14 E(K) =  9.174E-02 E(ENTH+SPEC) =  5.346E-06  E(SUM) =  1.043E+00
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  4.61421E-03
      INNER  1 : E(ENTH+SPEC) =  1.07726E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.99044E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  1.08450E-04  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  2.16836E-05  ALPHA =  1.00000E+00
      INNER  5 : E(ENTH+SPEC) =  1.41765E-06  ALPHA =  1.00000E+00
ITER 15 E(K) =  8.358E-02 E(ENTH+SPEC) =  1.418E-06  E(SUM) =  7.879E-01
        DAMP =  1.000E+00
      INNER  0 : E(ENTH+SPEC) =  4.58525E-03
      INNER  1 : E(ENTH+SPEC) =  2.89594E-03  ALPHA =  1.00000E+00
      INNER  2 : E(ENTH+SPEC) =  4.48525E-04  ALPHA =  1.00000E+00
      INNER  3 : E(ENTH+SPEC) =  2.84930E-05  ALPHA =  1.00000E+00
      INNER  4 : E(ENTH+SPEC) =  2.14820E-06  ALPHA =  1.00000E+00
```



Convergence Strategy

Strategy

There are two ways of designing a process model

1) One way is to make it so simple that there are obviously no problems
2) The other way is to make it so complicated that there are no obvious problems

The first is far more difficult

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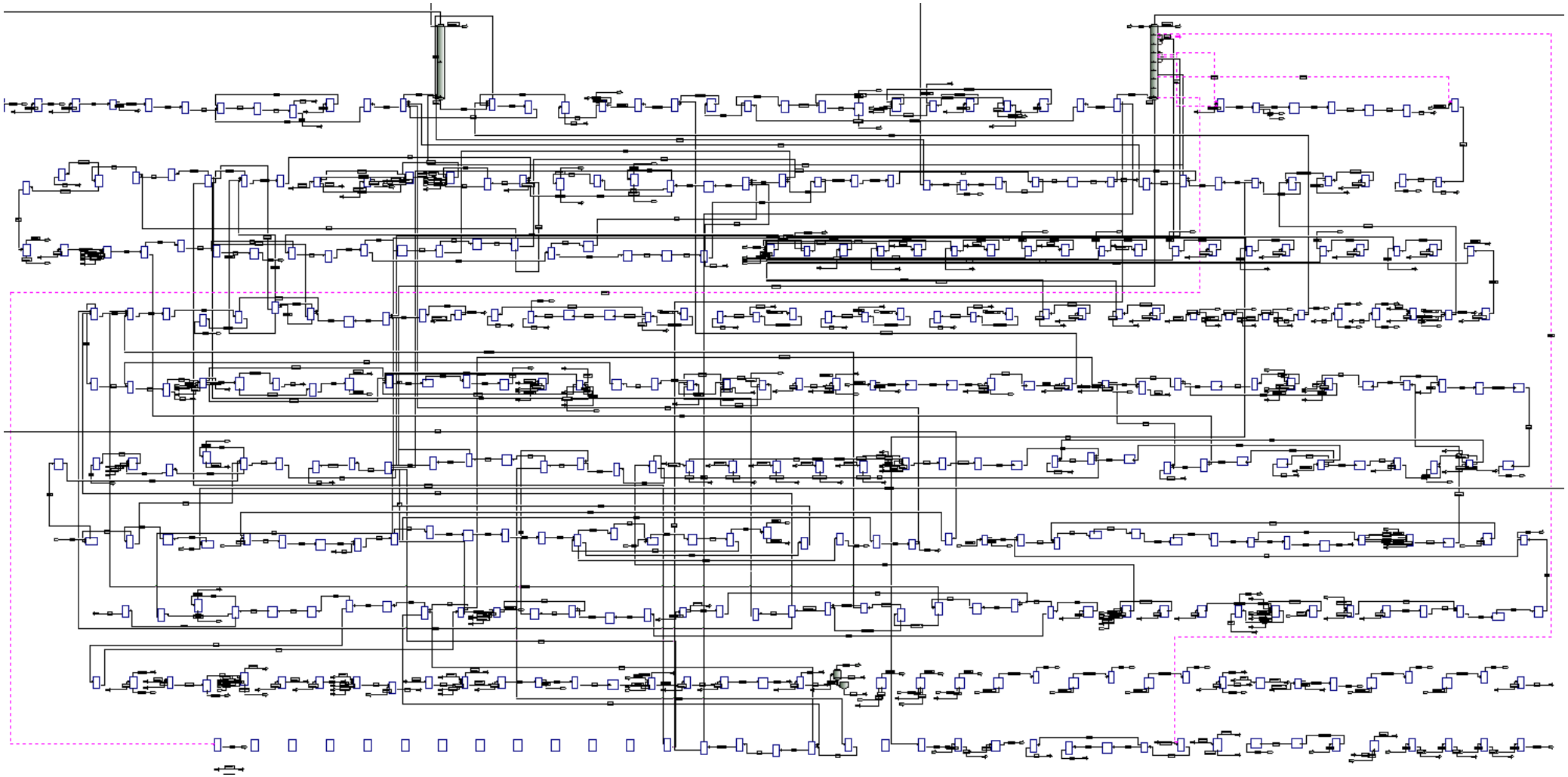
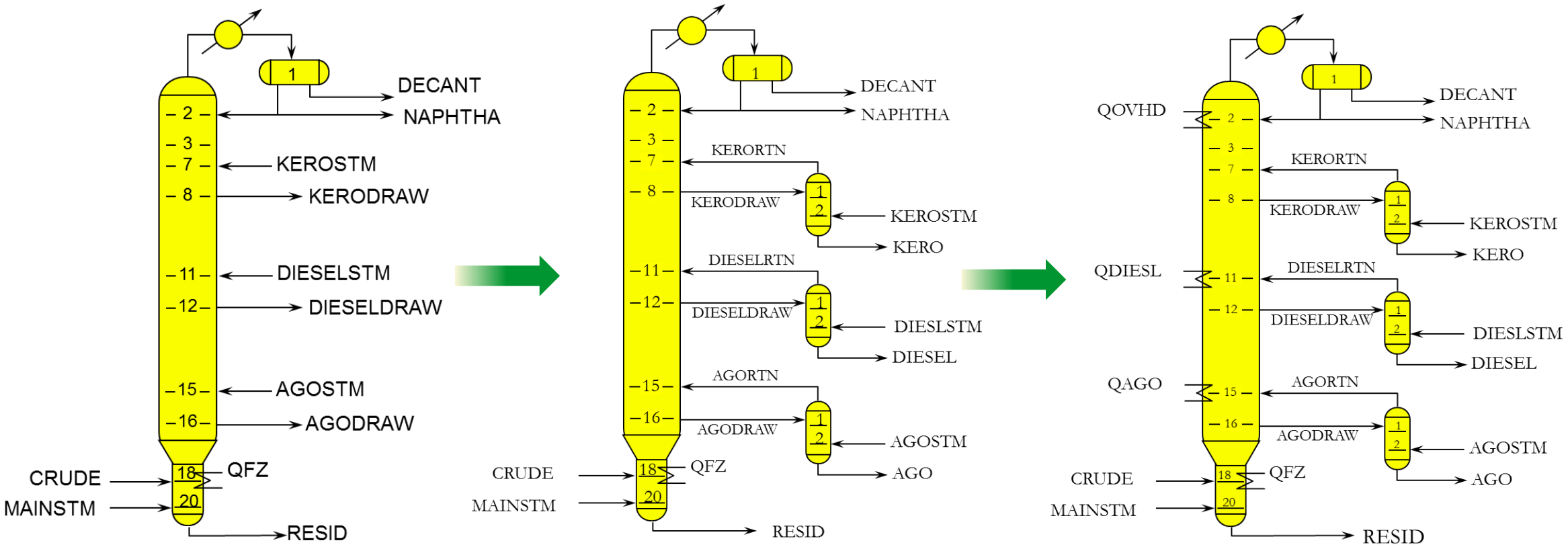
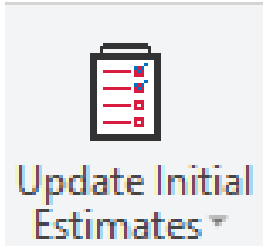
Model Complexity

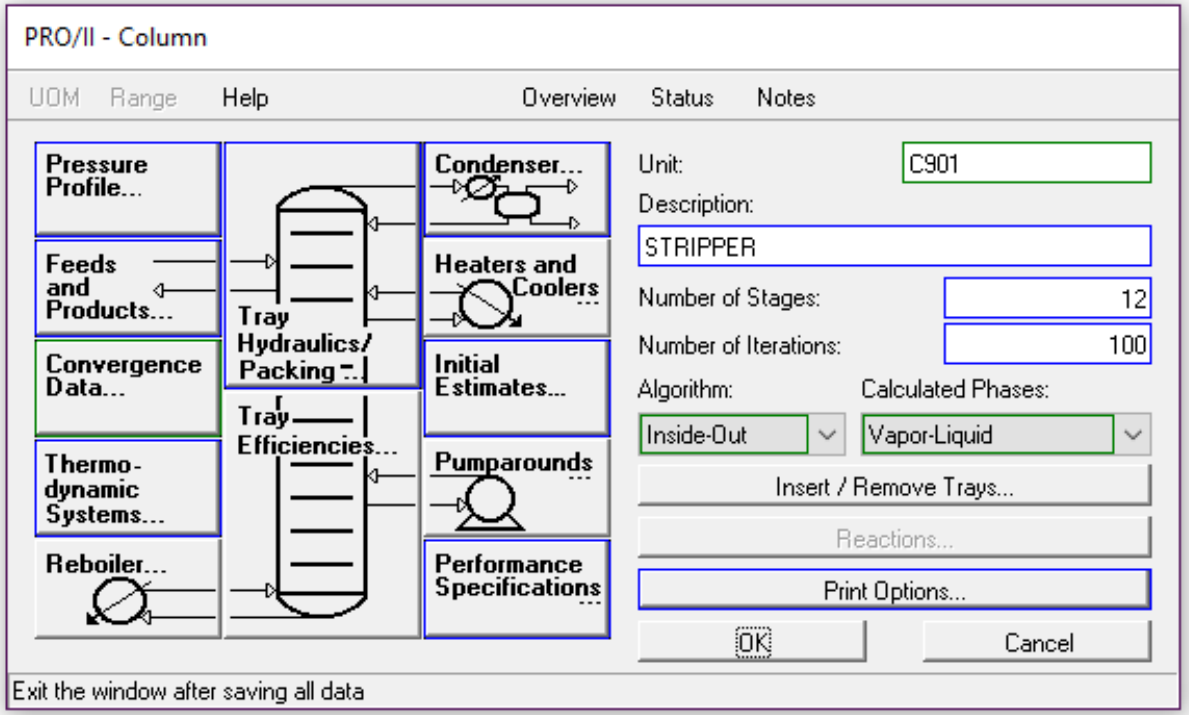


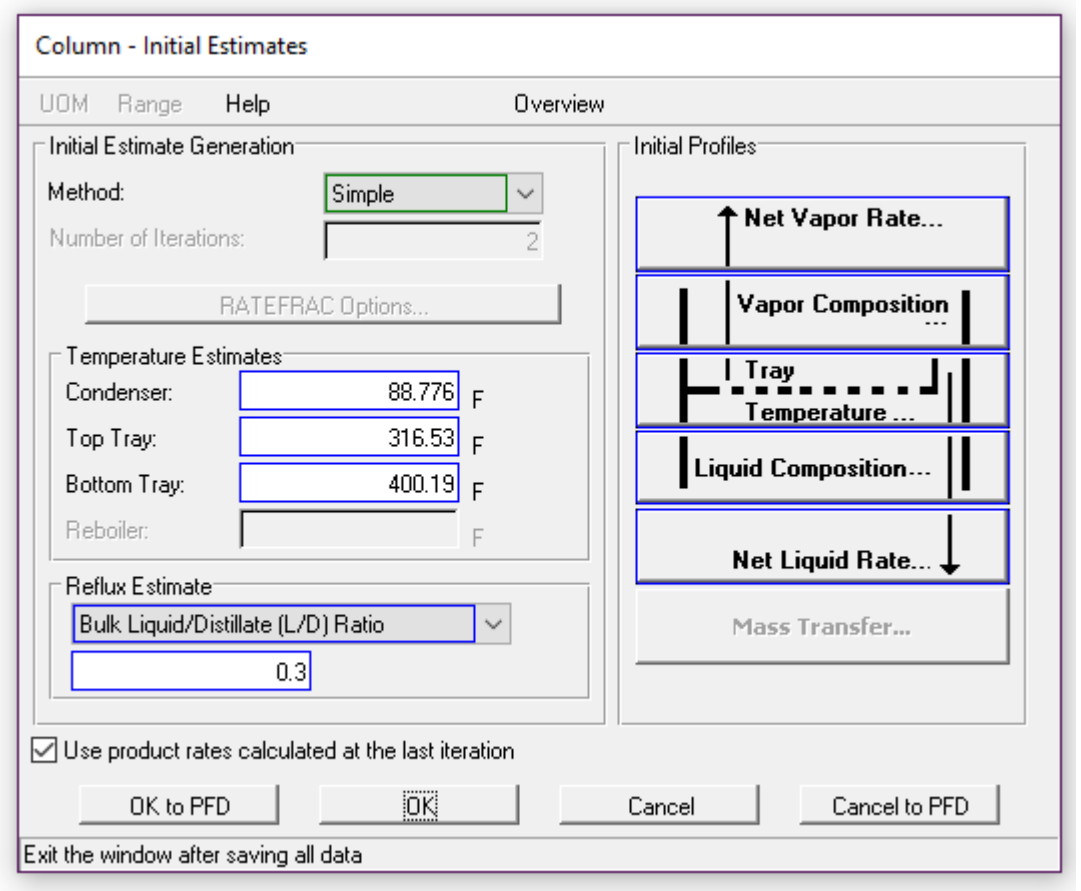
Start Slowly



Provide Estimates







Strategy

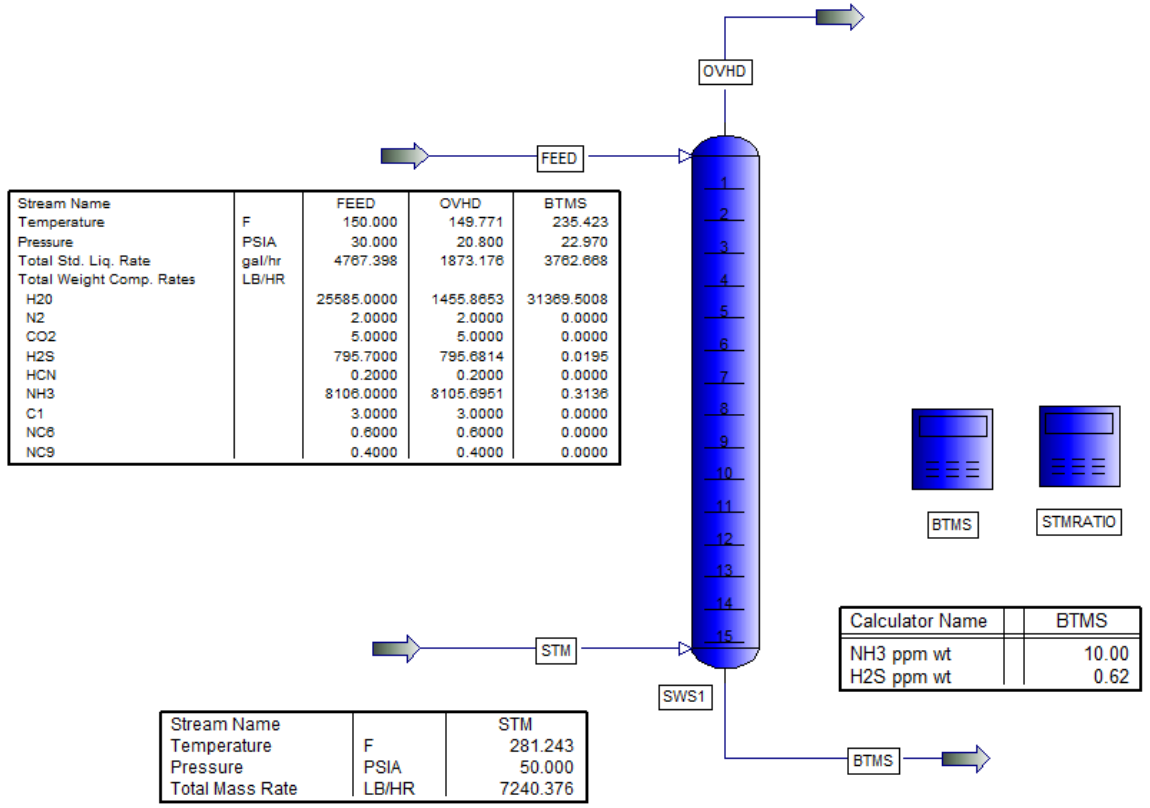
If the column is not solving, provide molar estimates

- Internally distillation algorithms converge on moles because VLE equations are written using moles (not mass or volume)

Product	Type of Product	Phase	Tray	Rate	
S2	Overhead	Vapor	1		lb-mol/hr
S3	Fixed Rate Draw	Liquid	1		lb-mol/hr
S4	Bottoms	Liquid	11		lb-mol/hr
S5					lb-mol/hr

Strategy

Use Stream / Unit Op Property Tables to facilitate convergence



Stream Name		FEED	OVHD	BTMS
Temperature	F	150.000	149.771	235.423
Pressure	PSIA	30.000	20.800	22.970
Total Std. Liq. Rate	gal/hr	4767.398	1873.176	3762.668
Total Weight Comp. Rates	LB/HR			
H20		25585.0000	1455.8653	31369.5008
N2		2.0000	2.0000	0.0000
CO2		5.0000	5.0000	0.0000
H2S		795.7000	795.6814	0.0195
HCN		0.2000	0.2000	0.0000
NH3		8106.0000	8105.6951	0.3136
C1		3.0000	3.0000	0.0000
NC6		0.6000	0.6000	0.0000
NC9		0.4000	0.4000	0.0000

Calculator Name	BTMS
NH3 ppm wt	10.00
H2S ppm wt	0.62

Stream Name		STM
Temperature	F	281.243
Pressure	PSIA	50.000
Total Mass Rate	LB/HR	7240.376

Calculator Name	STMRATIO
Steam/Feed Ratio, lb/gal	1.52

Strategy

Check the Column Profile

COLUMN SUMMARY

TRAY	TEMP DEG F	PRESSURE PSIG	NET FLOW RATES LIQUID LB-MOL/HR	NET FLOW RATES VAPOR LB-MOL/HR	NET FLOW RATES FEED LB-MOL/HR	NET FLOW RATES PRODUCT LB-MOL/HR	HEATER DUTIES MM BTU/HR
1C*	110.0	5.30	0.0			2832.0L	-79.2914
						1032.7W	
2	269.3	8.50	8363.0	3864.7	6337.7P		-49.9998
3	299.7	8.75	1956.0	5890.0		6337.7P	
4	324.2	9.00	1929.5	5820.7			
5	338.2	9.25	1735.8	5794.2			
6	346.5	9.50	1563.2	5600.6			
7	355.0	9.75	1352.6	5427.9	413.1V		
8	367.9	10.00	4.2	4804.3		1122.1L	
9	389.1	10.25	5650.1	4578.0	4368.5P		-49.9998
10	423.8	10.50	1182.0	5855.4		4368.5P	
11	460.2	10.75	944.2	5755.8	385.9V		
12	481.9	11.00	124.7	5132.1		601.3L	
13	500.0	11.25	4082.9	4914.0	3413.8P		-39.9995
14	528.4	11.50	647.9	5458.3		3413.8P	
15	560.5	11.75	484.7	5437.1	129.9V		
16	574.0	12.00	0.0	5144.0		269.8L	
17	585.9	12.25	0.9	4929.2			
18	581.4	12.50	2610.2	4930.1	6548.6M		147.5795
19	580.0	12.75	2383.6	990.8			
20	576.3	13.00		764.2	555.1V	2174.5L	

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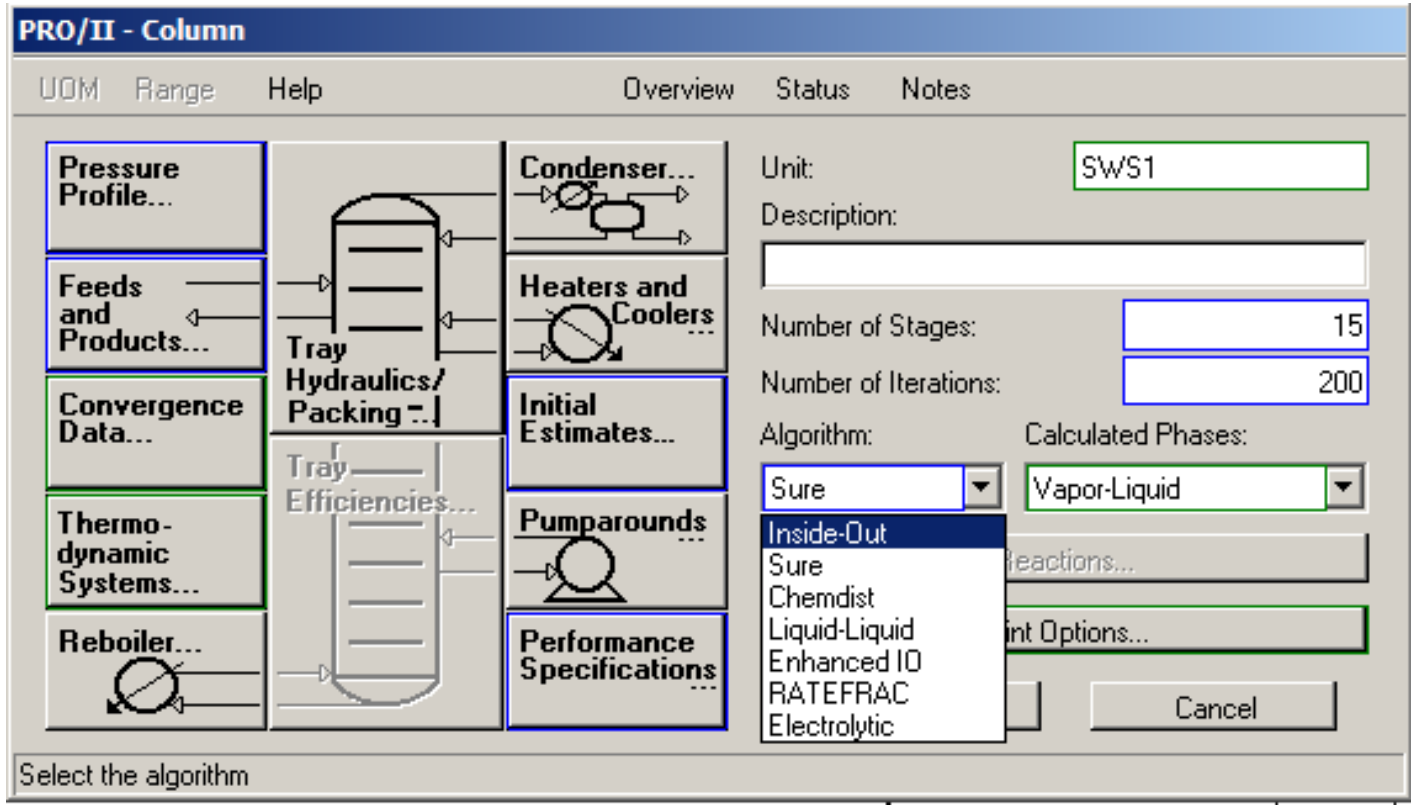
Strategy

Use an Appropriate Algorithm



SWS

Conclusions and Takeaways

- Start off simple
- Ensure you have the correct setup (IEG, Algorithm, Estimates, and Iterations)
- Examine the output for oscillations or divergence – use damping
- Ensure that all trays have vapor and liquid
- 1 800 SimSci1
- support.simsci@aveva.com

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Questions?

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