Incorporating Reality Into Process Simulation

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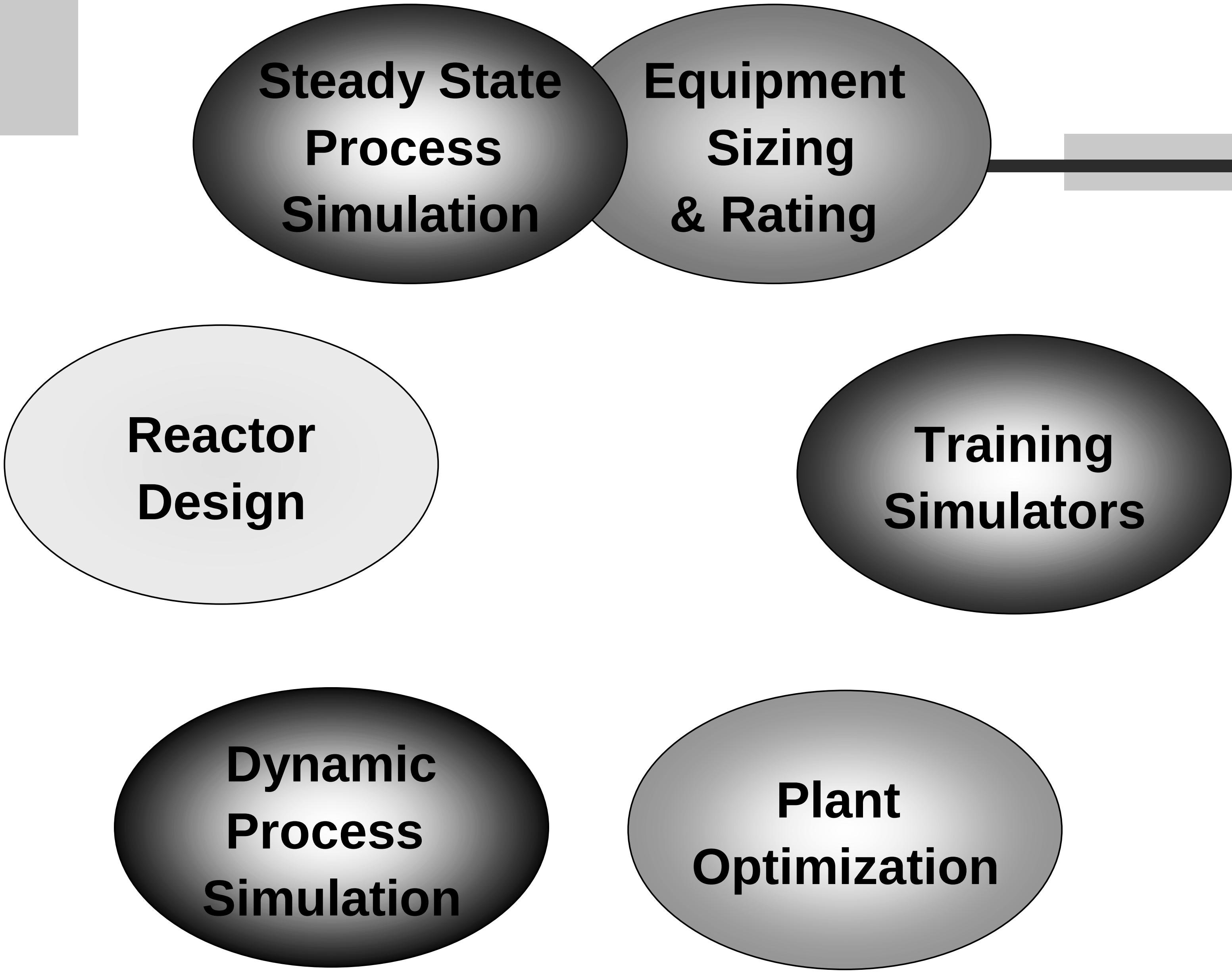
Levels of Reality in Process Simulation

1. Data Accuracy and Comprehensiveness
   - Physical Properties
   - Phase Properties (BIP's)
   - Chemical Properties
2. Equilibrium Models
   - Phase (VLE, LLE, SLE)
   - Chemical Reaction (Gibbs or Emperical)
3. Rate Models
   - Reaction
   - Mass Transfer
   - Heat Transfer
   - Momentum Transfer (pressure drops)

Levels of Reality in Process Simulation

4. Mechanical Considerations
   - Pump and Compressor performance curves
   - Valve Geometry
   - Solids UnitOps
5. Time Dependence
   - Holdups
   - Transients inputs and fluctuations
   - Signal delays
   - Control response

Historically,



Historically,

Over time these gaps began to close:

i. Faster computers

ii. Better software technology

iii. Improved numerical techniques

iv. Better engineering models

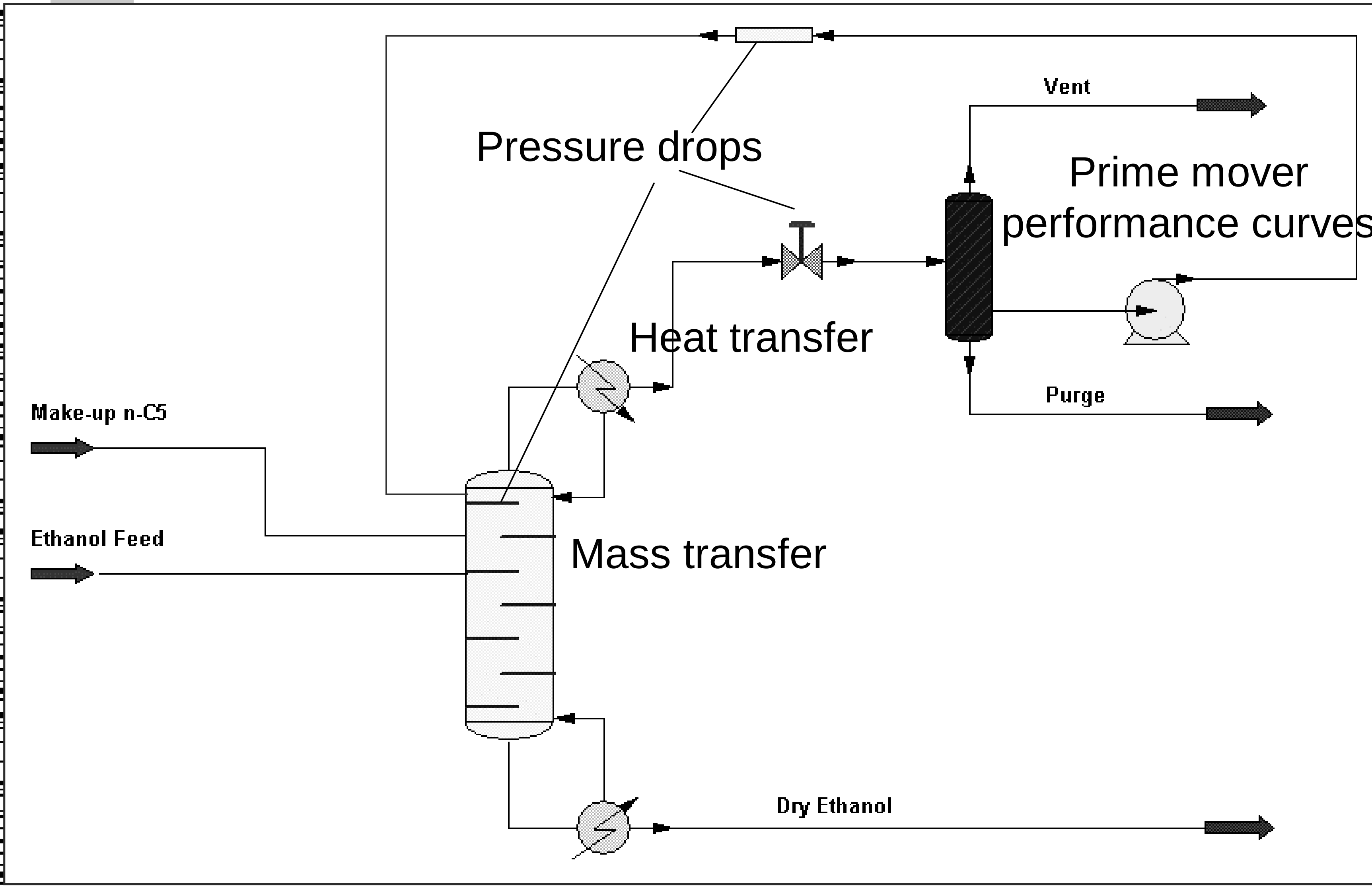
v. Cumulative effort

Historically,

These things resulted in the following developments:

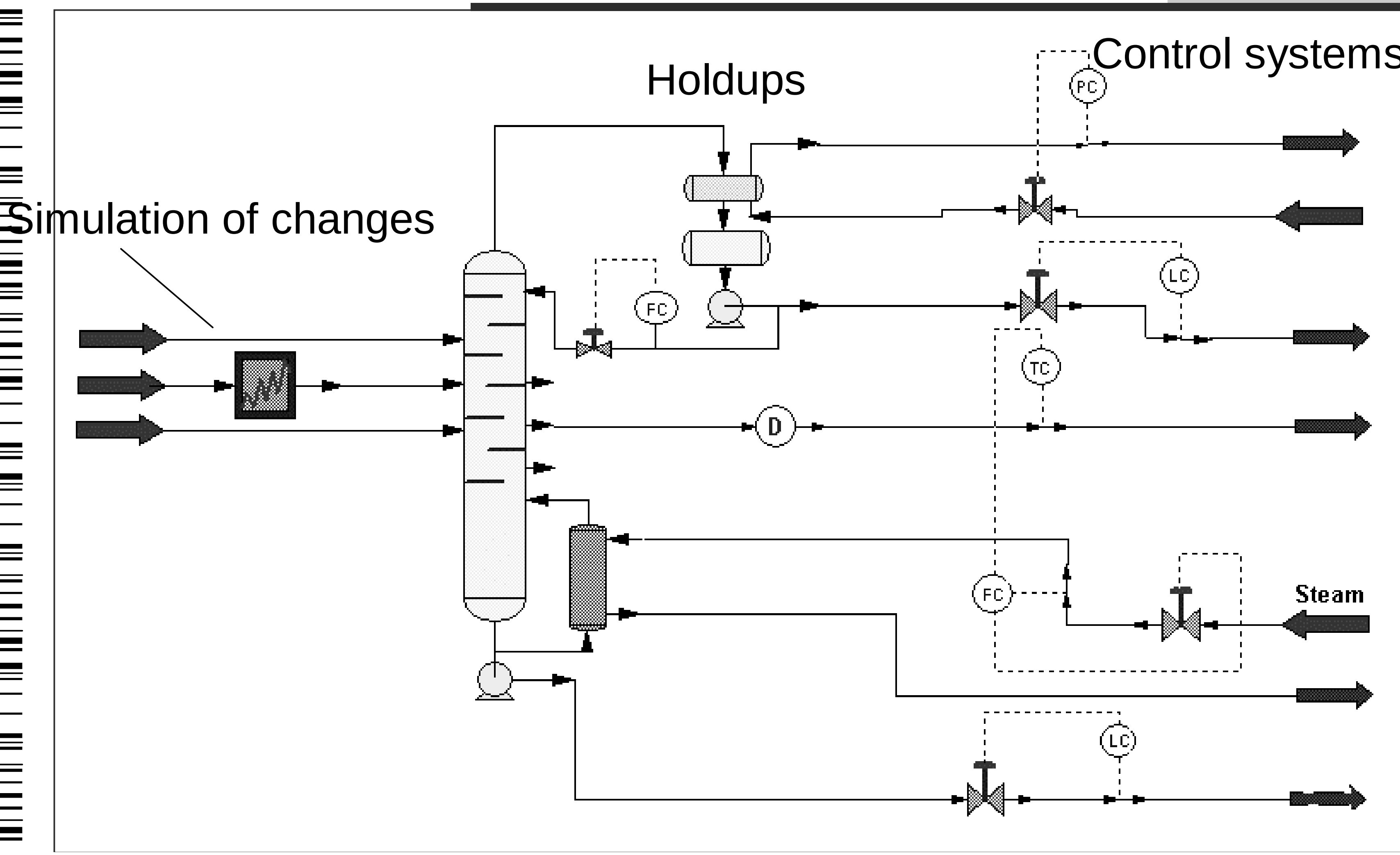
- Dynamic Simulation
  - required equipment parameters such as geometry, Cv, PIDC, etc
- Mass transfer
  - required column geometries
- Numerical techniques
  - full or quasi equation solving permitted integration of piping, valves, etc.
- Better software and faster computers
  - integration of many components or models
  - customization
  - communications

Now simulations can be more realistic:

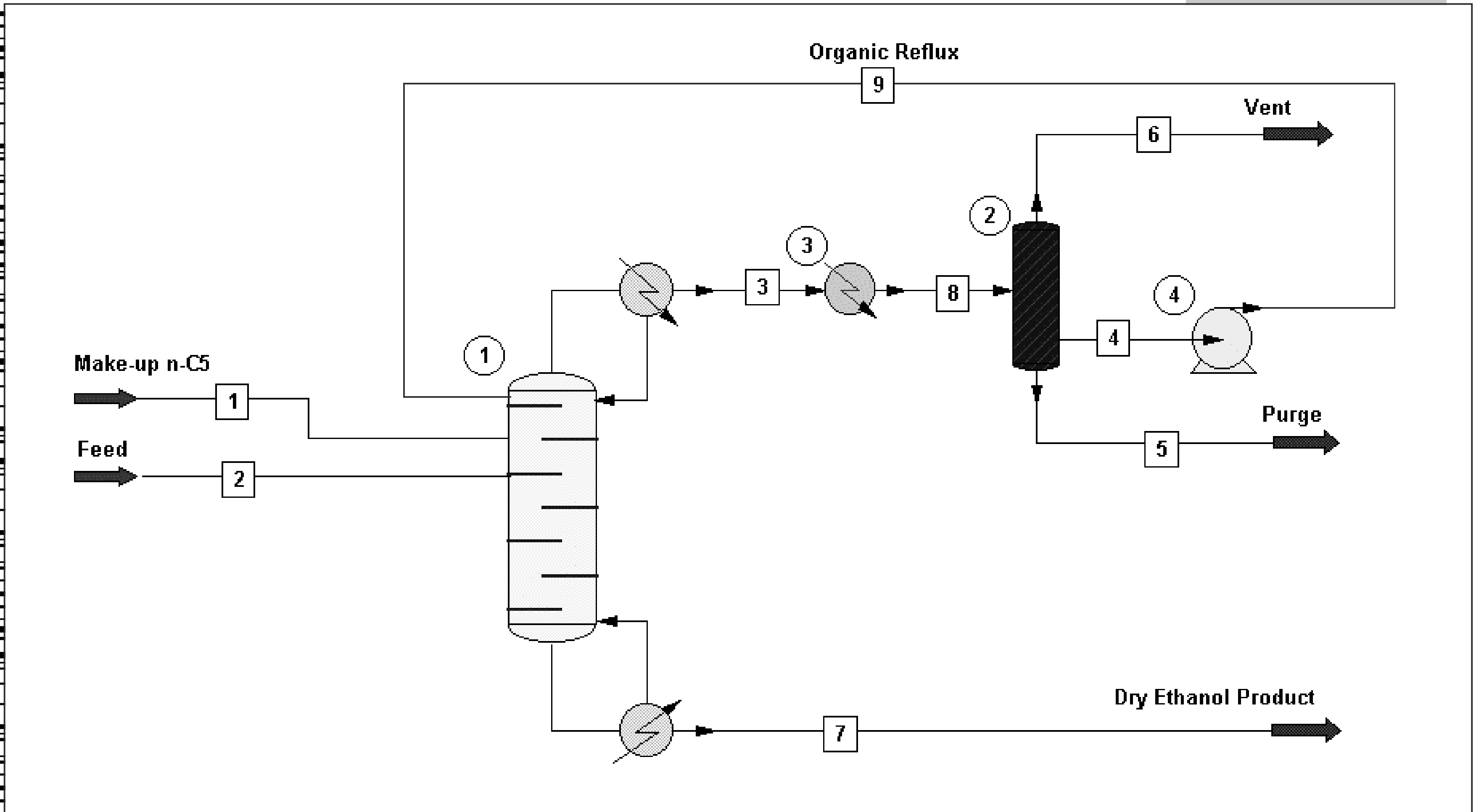


Now simulations can be more realistic:

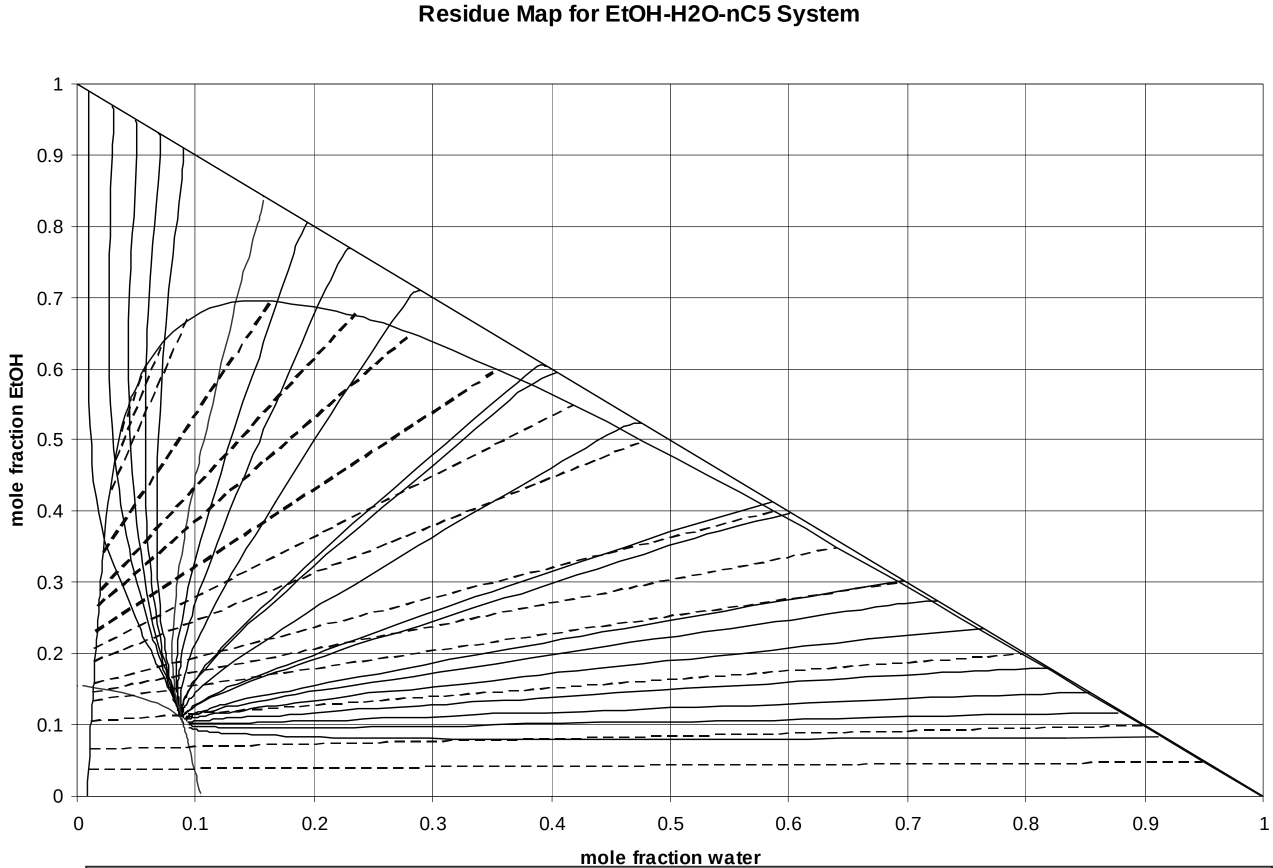
Dynamic considerations



Azeotropic Distillation Example:



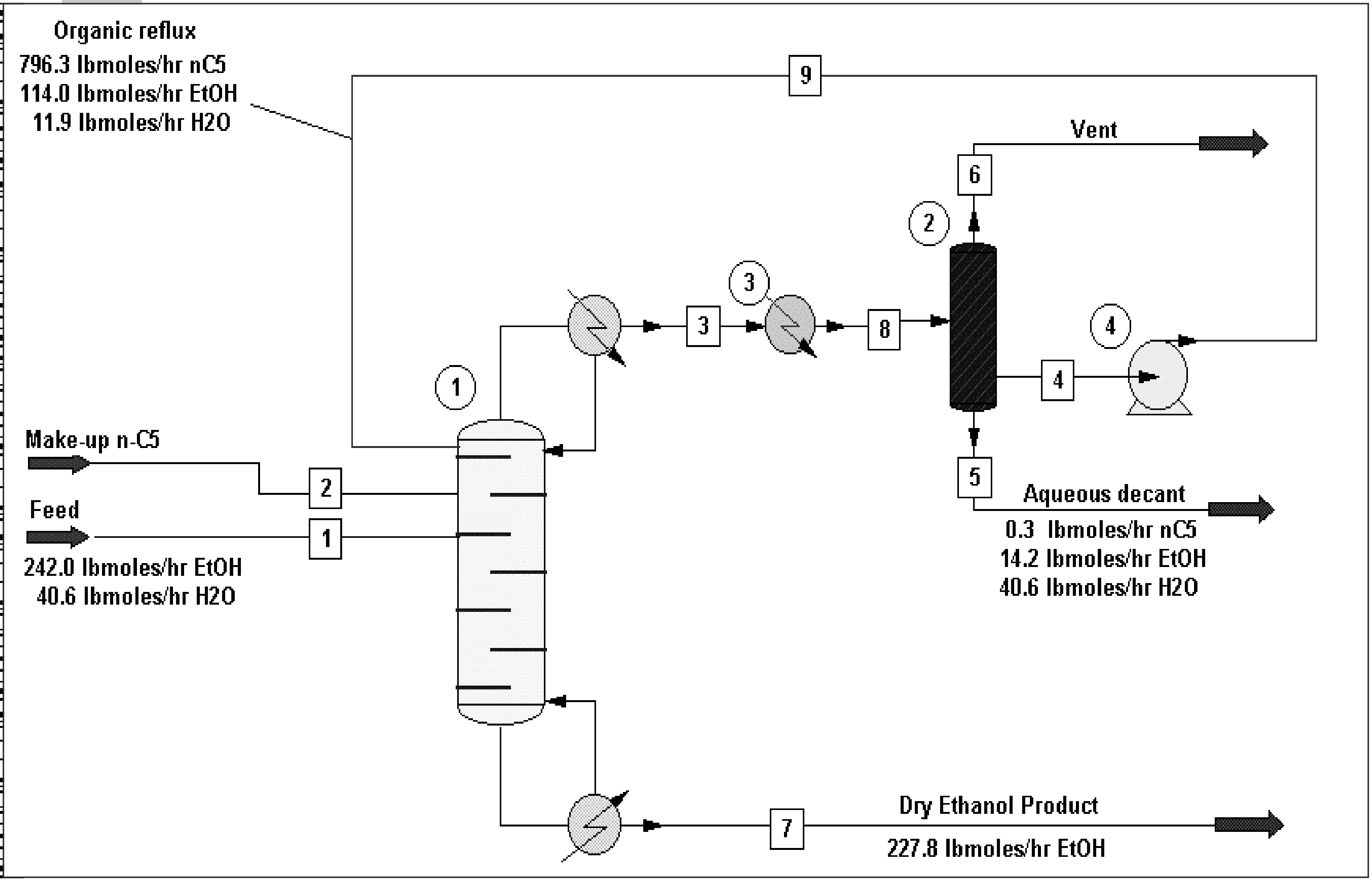
Residue Curve Map for Azeotropic System



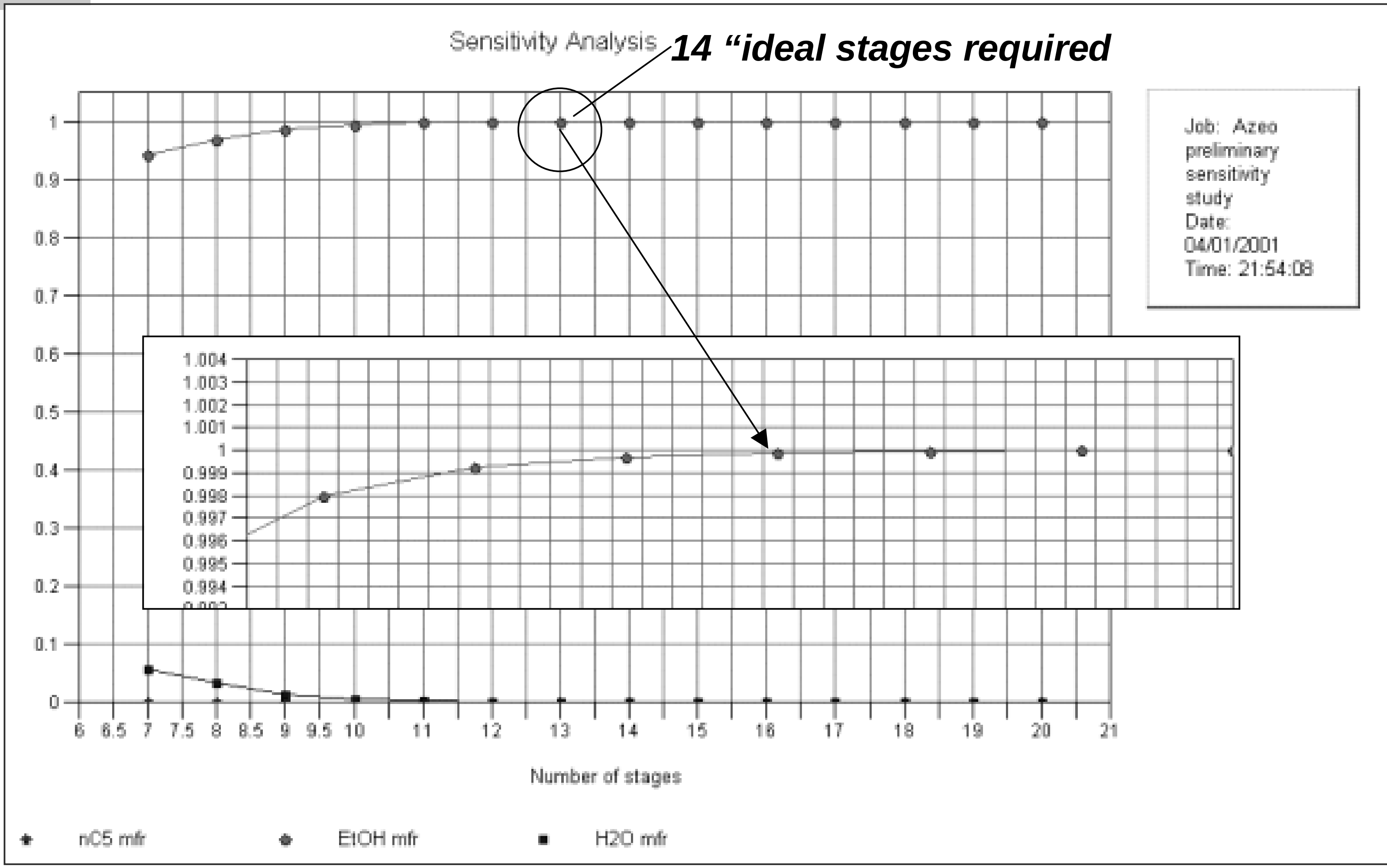
From this map we can verify our thermodynamic model.

	Miscible/immiscible	Azeotrope composition, mole%	Azeotrope temperature, F
Ethanol-water	Miscible	90.4 .v. 90.8 EtOH	172.8 .v. 173.1
Ethanol-npentane	Miscible	92.4 .v. 92.2 nC_5	93.7 .v. 95.5
npentane-water	Immiscible	94.6 .v. 94.6 nC_5	94.3 .v. 93.8
Ethanol-water-npentane	immiscible	4.4,6.1,89.5 .v. 4.9,5.4,89.7	92.1 .v. 93.2

Preliminary Material Balance prepared from Residue Map



Sensitivity analysis using equilibrium stages:



The Early History of Distillation Calculations

1. Concept of equilibrium stage introduced by Sorel in 1893.
2. McCabe-Thiele diagrams for number of theoretical stages in 1925
3. Lewis-Matheson and Thiele-Geddes methods for rigorous (tray-by-tray) multicomponent distillation in 1930's. Not generally used until the appearance of computers in the 1950's.

Mass Transfer in Distillation Calculations (cont.)

In all of these methods the departure from thermodynamic equilibrium is accounted for by using empirical factors:

(i) stages efficiencies for trays

(ii) HETP for packing

Trays: Stage efficiencies can vary $-\infty$ to $+\infty$. Vary with component, stage, conditions, etc.

Packing: HETP varies not only with size and type of packing, but also from one component to another and strongly from point to point in a column to another.

These phenomena are especially true for non-ideal mixtures, operating at extreme conditions.

Mass Transfer in Distillation Calculations (cont.)

The rate based approach:

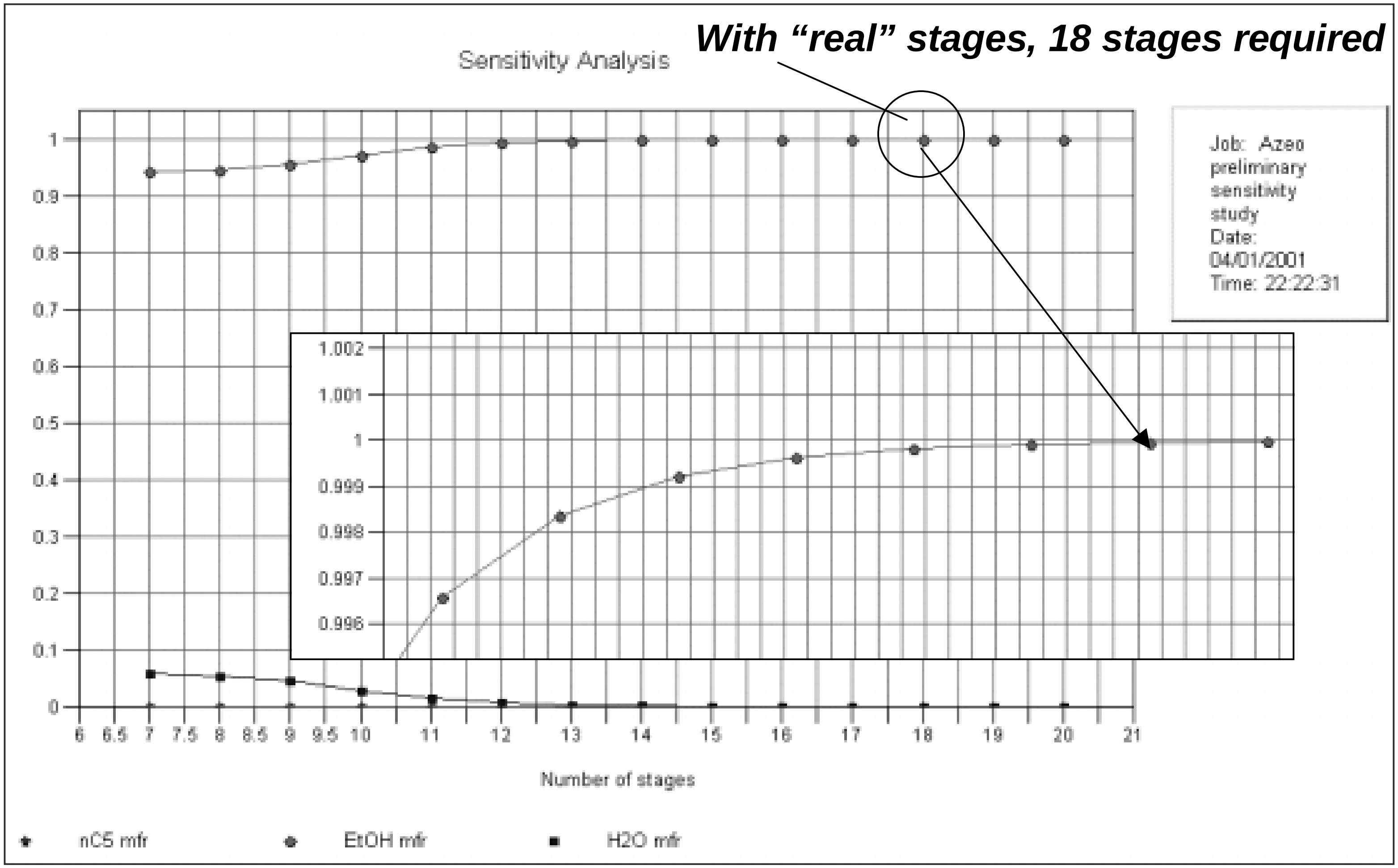
1. Is more complex.
2. Has shorter application history.
3. Is completely predictive (based on component physical properties and BIPs), so avoids stage efficiencies and HETP.
4. Is at least as accurate as the equilibrium method.
5. Is the only method which can guarantee the accuracy of simulations involving simultaneous mass transfer and chemical reactions.

With tray layout and mass transfer calculations included:

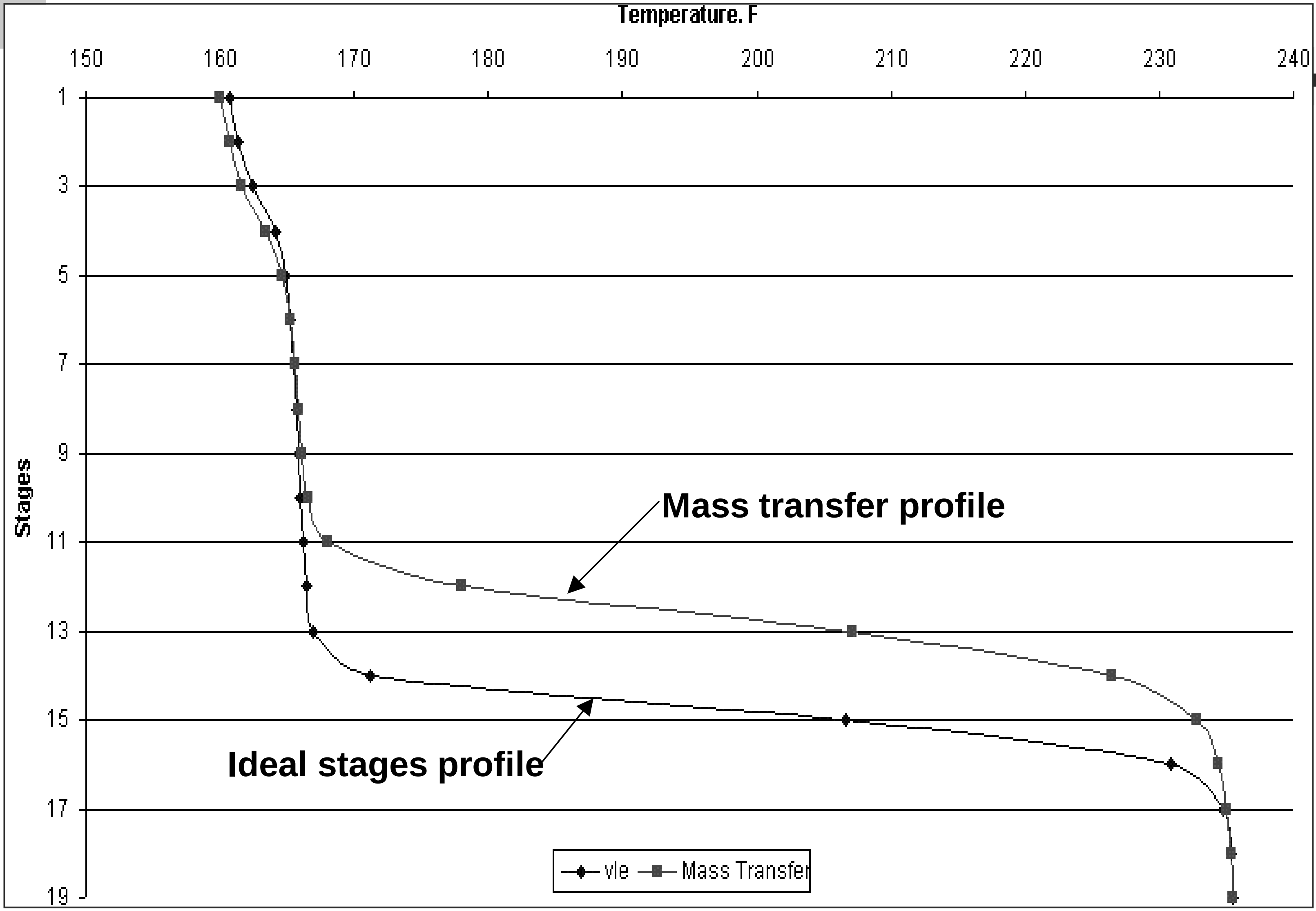
```
              Equip.   1   Tray No.   1

Tray Loadings                        Vapor              Liquid
                                 64176.582 lb/h      62944.359 lb/h
                                124535.495 ft3/hr     1723.614 ft3/hr
Density                              0.515 lb/ft3       36.519 lb/ft3
System factor                      ................      1.000
Valve type     :  V-1
Valve material :  S.S.
Valve thickness, gage              ................     12.000
Deck  thickness, gage              ................     14.000
Tower internal diameter,  ft       ................      6.000
Tray spacing,  in                  ................     24.000
No. of tray liquid passes          ................          1
Downcomer dimension,            Width in   Length in    Area ft2
               Side              10.750     51.320       2.642
Avg. weir length   in              ................     51.320
Weir height,  in                   ................      2.000
Flow path length   in              ................     50.500
Flow path width   in               ................     65.559
Tray area, ft2                     ................     28.274
Tray active area ft2               ................     22.991
% flood                            ................     47.900
Hole area ft2                      ................      4.368
Approx # of valves                 ................        342
Tray press loss,  in               ................      3.977
Tray press loss, psi               ................      0.084
Dry press drop,  in                ................      2.138
Downcomer clearance  in            ................      3.000
Downcomer head loss  in            ................      0.130
Downcomer backup  in               ................      7.205
Downcomer residence time, sec      ................      3.313
Liquid holdup    ft3               ................      5.110
Liquid holdup     lb               ................    186.605
Design pressure, psia              ................     47.558
Joint efficiency                   ................      0.850
Allowable stress psia              ................  13700.000
```

Sensitivity analysis using mass transfer (rate based) method:



Temperature profiles under “ideal” and “real” conditions:



Heat transfer:

In conventional simulations, heat exchangers are simulated by making two types of specifications:

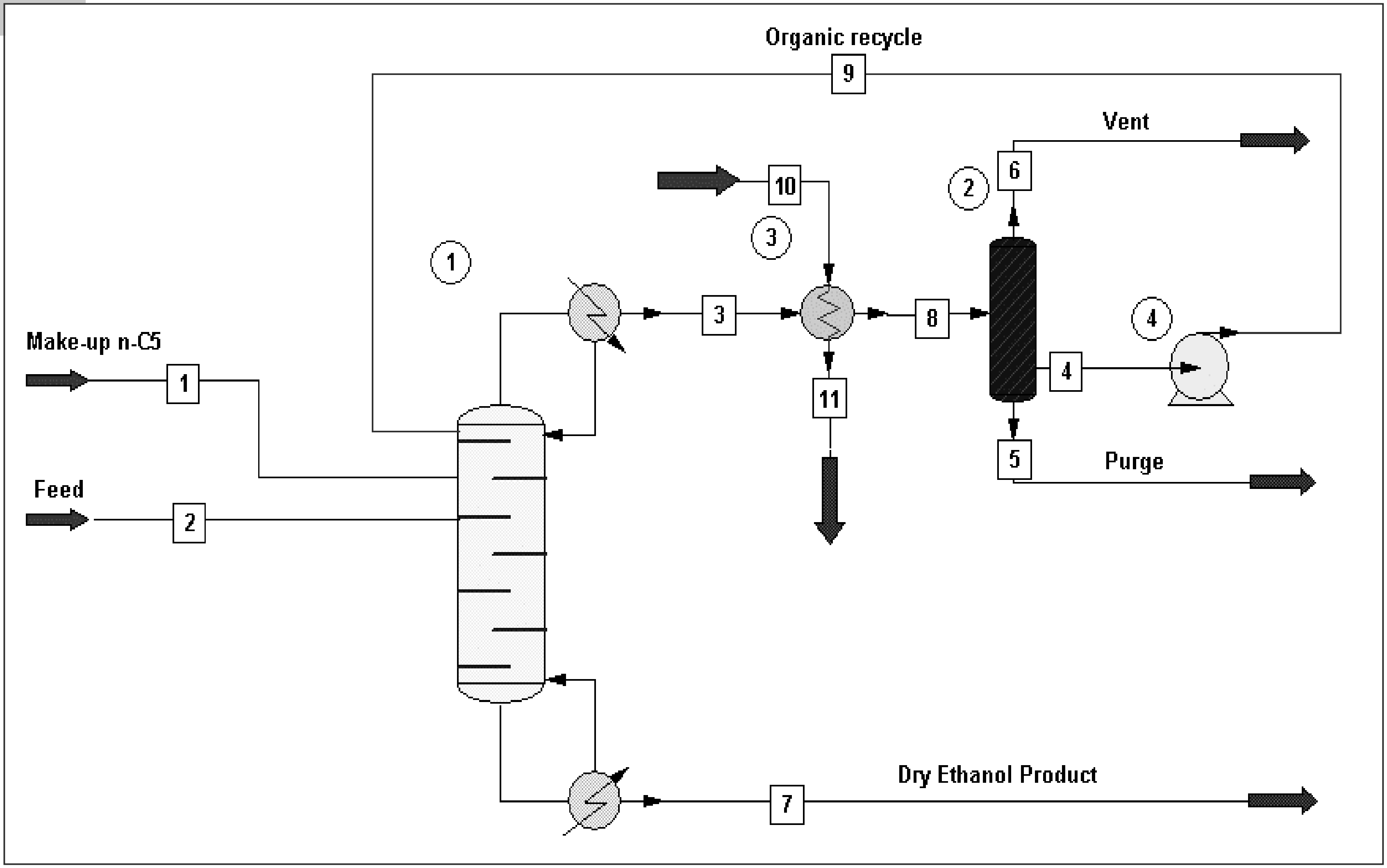
- Thermodynamic specs – T,Q,VF,…
- “Rating” specs – U*A (used frequently in dynamics)

This approach will not account for changing conditions which affect:

- film coefficients
- pressure drops
- varying outlet temperatures
- possible unexpected phase changes

Rigorous rating is done after the simulation.

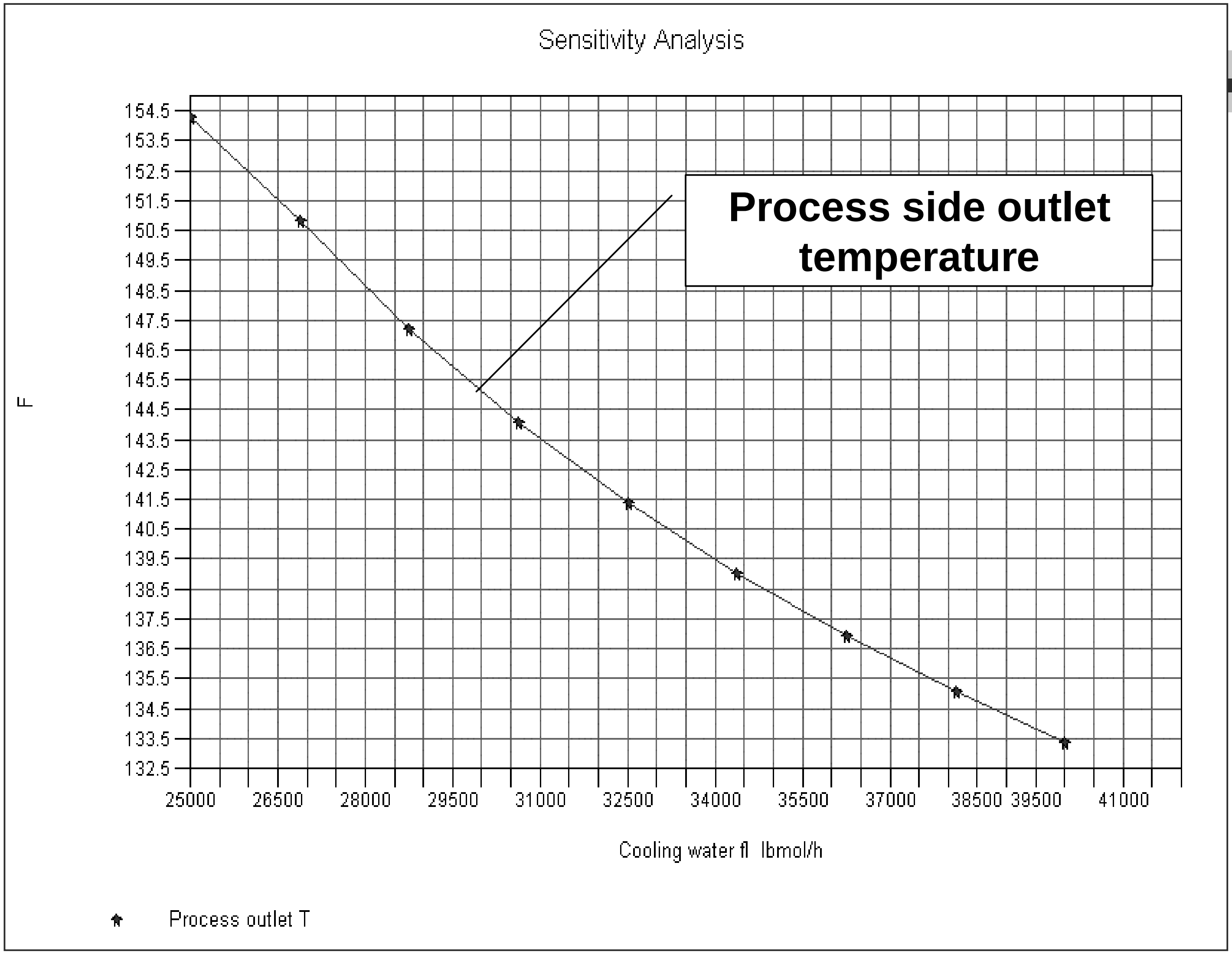
Heat transfer:



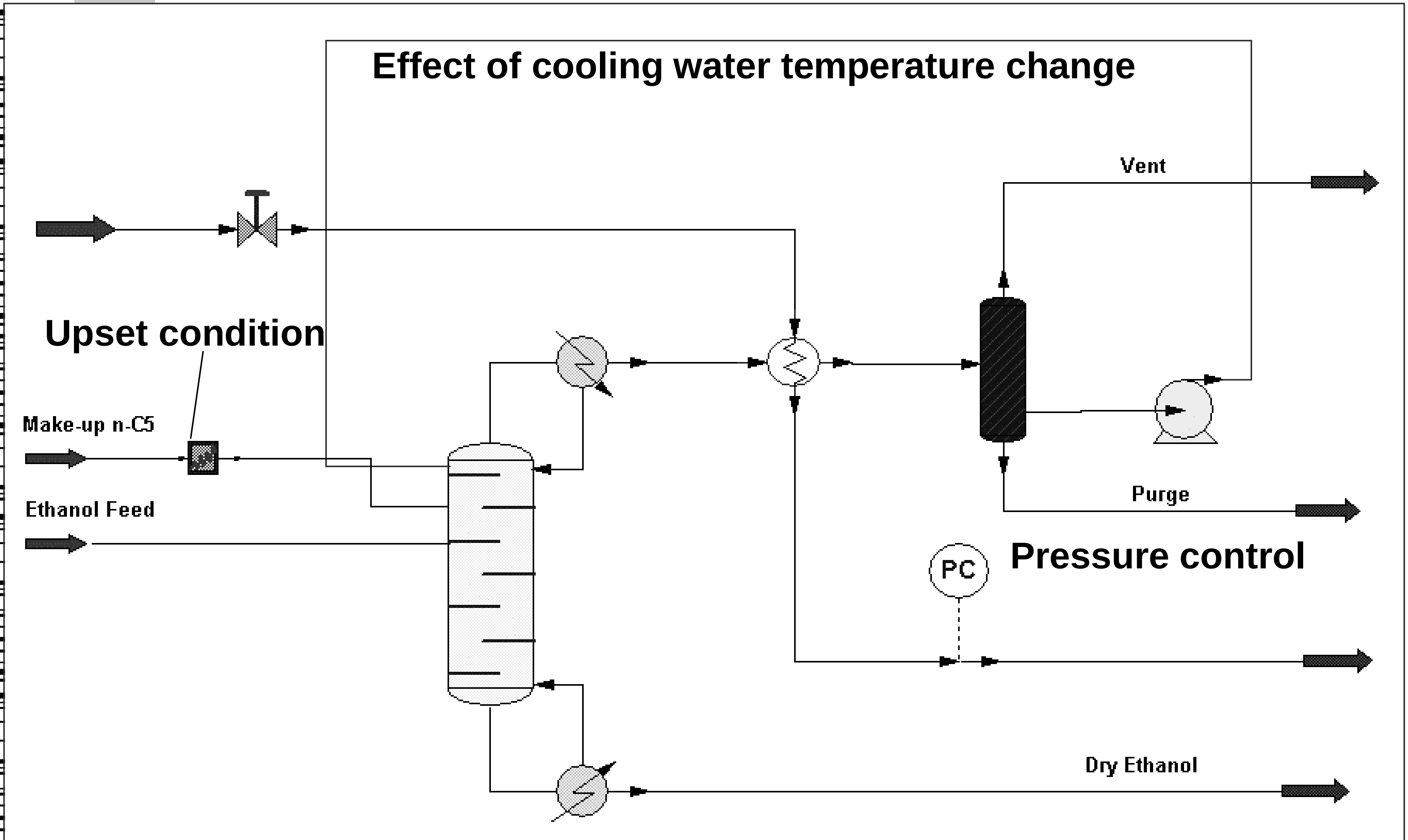
Heat transfer:

	TEMA SHEET			
1	----------			
2	Customer		Ref No.	
3	Address		Prop No.	
4	Plant Loc.		Date	Rev
5	Service of Unit		Item	
6	Size 27.0in x 20.0ft Type AEL (Hor/Vert) H Connected in 1 Para 1 Seri			
7	Surf/Unit 2572.2/2536.0 ft2; Shell/Unit 1.000000 Surf/Shell 2572.2/2536.0 ft2			
8	PERFORMANCE OF ONE UNIT			
9	Type of Process	Horiz Cond	Sensible	
10	Fluid Allocation	Shell Side	Tube Side	
11	Fluid Name			
12	Flow	64329.0	229691.2	lb/h
13	Liquid	0.0	229691.2	lb/h
14	Vapor	64329.0	0.0	lb/h
15	NonCondensable	0.00000	0.00000	lb/h
16	Steam	0.0	0.0	lb/h
17	Evap/Cond	64329.0	0.0	lb/h
18	Density	0.507/36.923	0.000/60.874	lb/ft3
19	Conductivity	0.011/0.059	0.000/0.361	Btu/hr-ft-F
20	Specific Heat	0.443/0.625	0.000/0.999	Btu/lb-F
21	Viscosity at Avg.	0.009/0.207	0.000/0.705	cP
22	Latent Heat	169.45	0.00	Btu/lb
23	Temperature(In/Out)	160.217/146.432	80.000/130.883	F
24	Operating Pressure	47.56	50.00	psia
25	Fouling Factor	0.001000	0.001000	hr-ft2-F/Btu
26	Velocity	6.18	0.76	ft/sec
27	Press Drop Allow/Calc	3.500/1.046	5.000/0.066	psi
28	Heat Exchanged 1.166e+001 MMBtu; MTD(Corrected): 48.91 F			
29	Transfer Rate, Service: 94.0 Clean: 115.8 Btu/hr-ft2-F			
30	CONSTRUCTION DATA/SHELL			Sketch
31		Shell Side	Tube Side	
32	Design/Test Press psia	0.000000/Code	0.000000/Code	
33	Design Temperature F	0.000	0.000	
34	No. Passes per Shell	1	1	
35	Corrosion Allowance in	0.000	0.000	
36	Connections IN ID in	12.000	12.000	

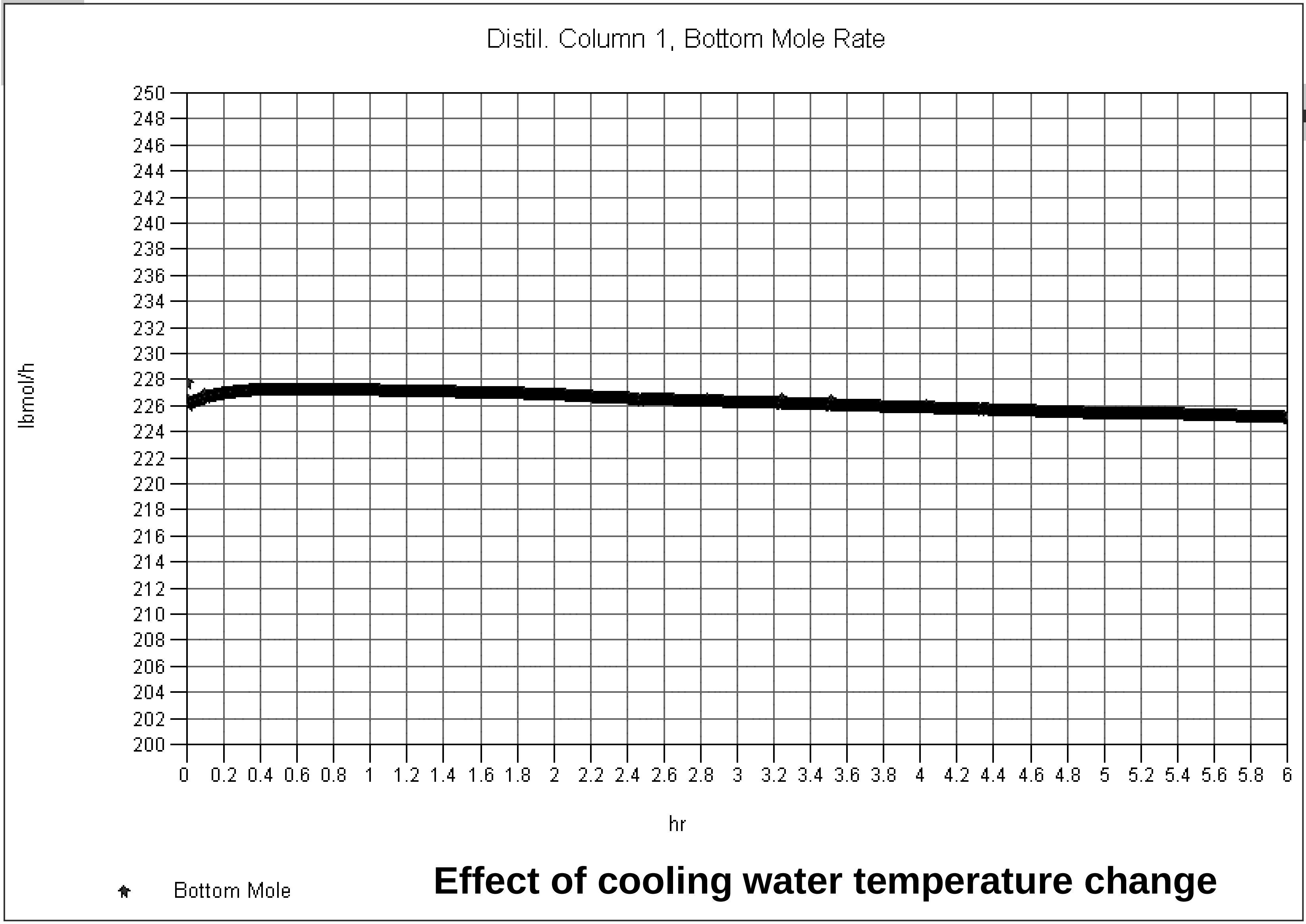
Heat transfer:



Dynamic Simulation

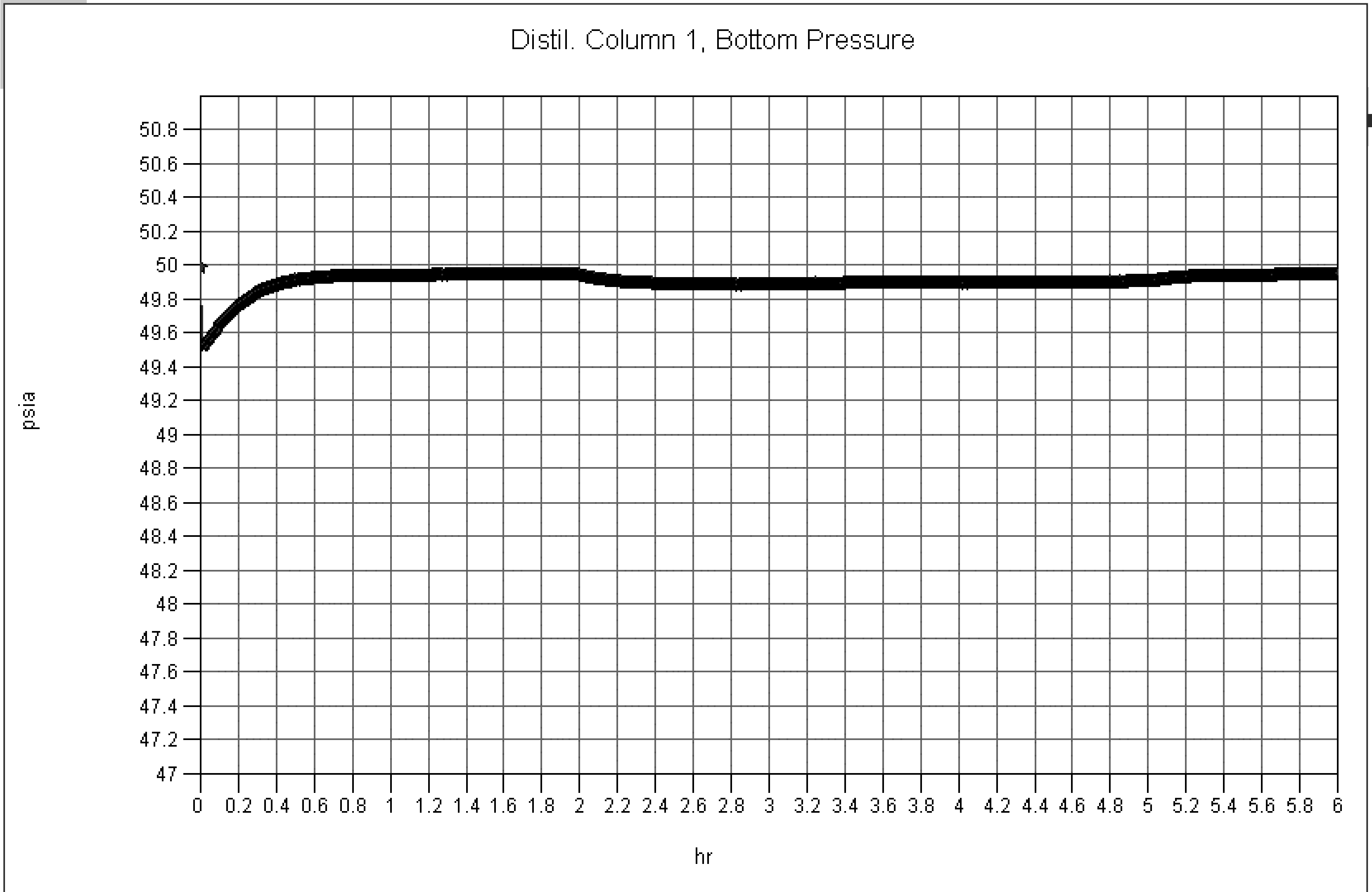


Dynamic Simulation



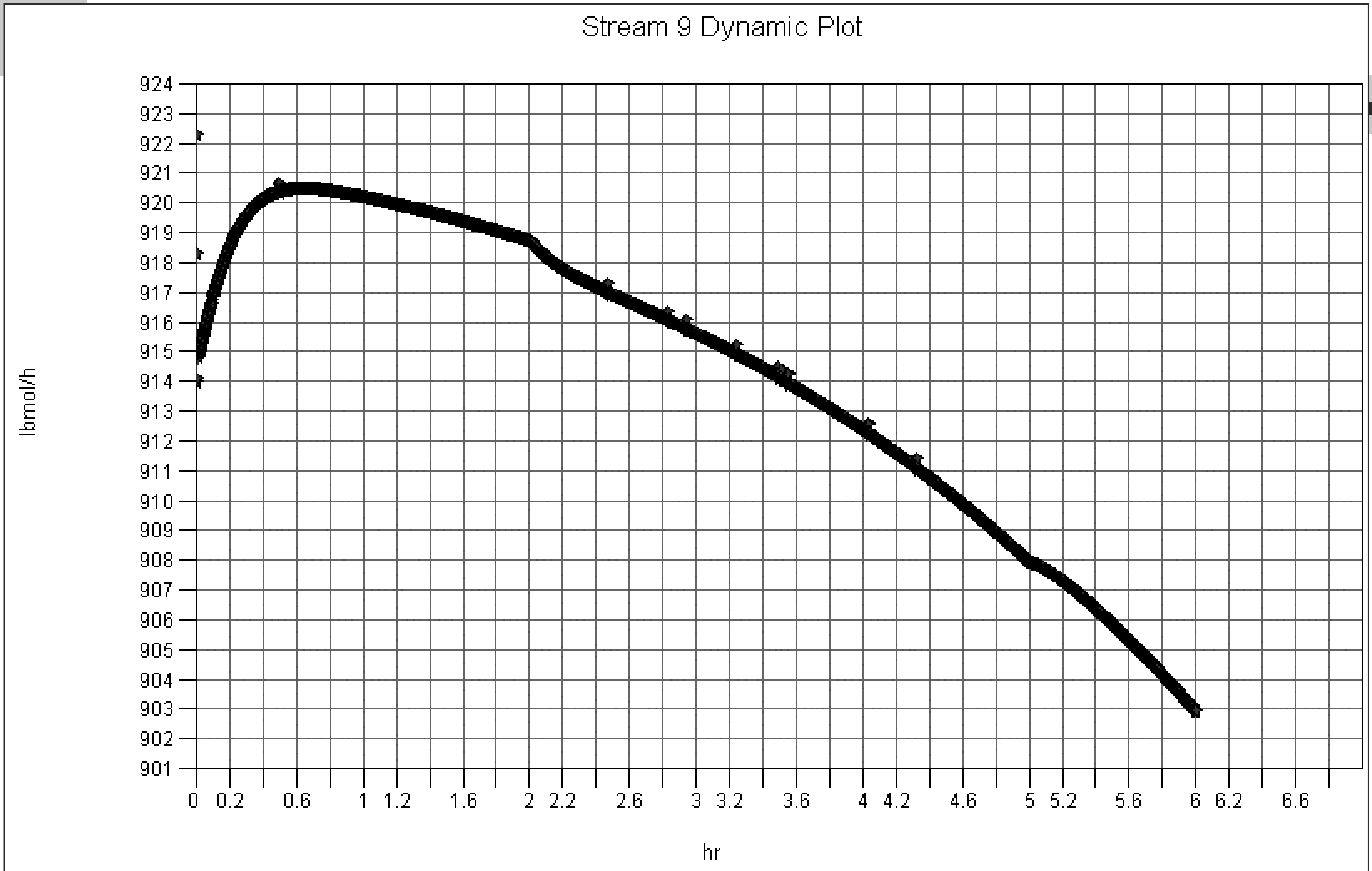
Effect of cooling water temperature change

Dynamic Simulation



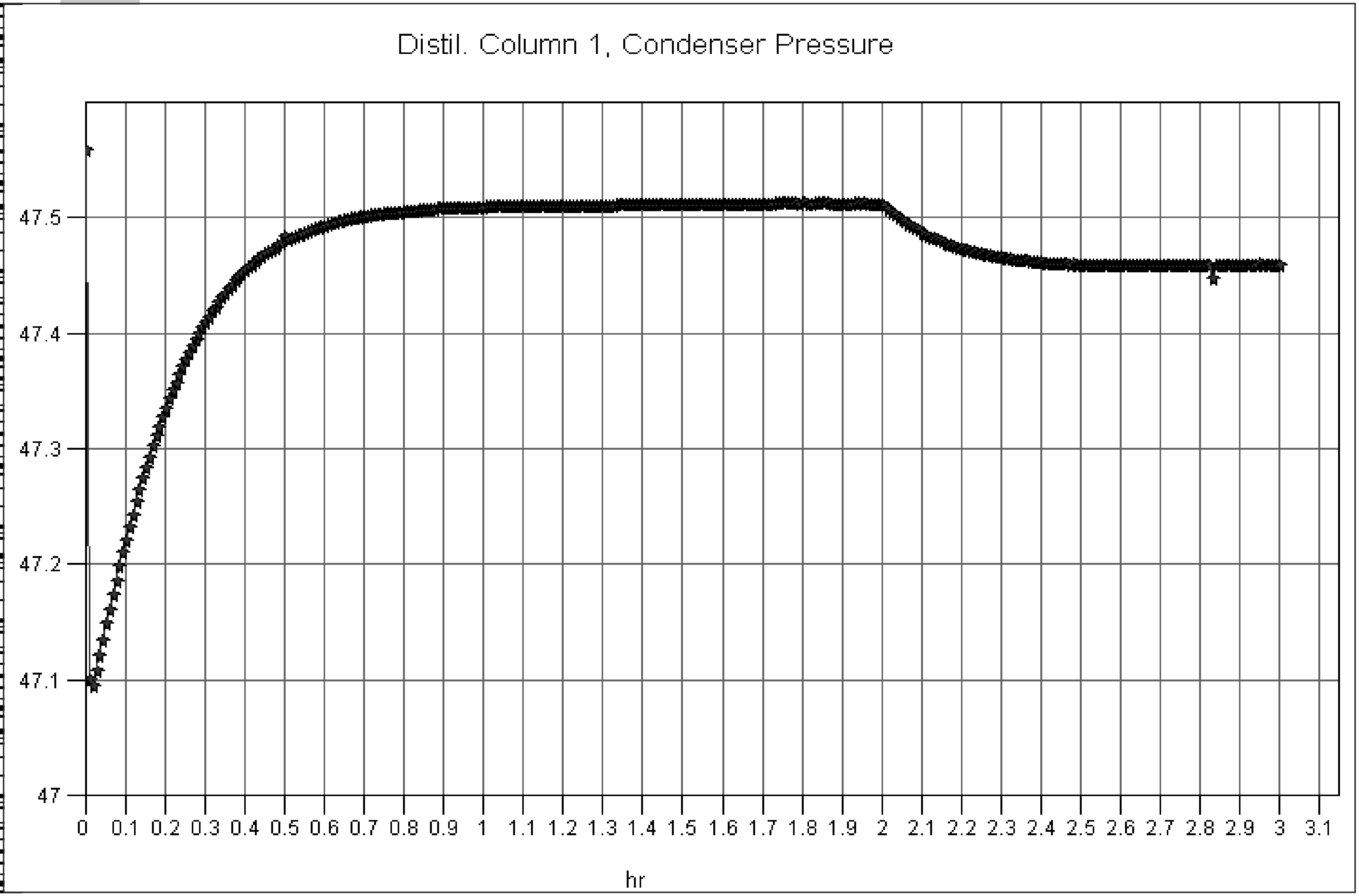
Effect of cooling water temperature change

Dynamic Simulation

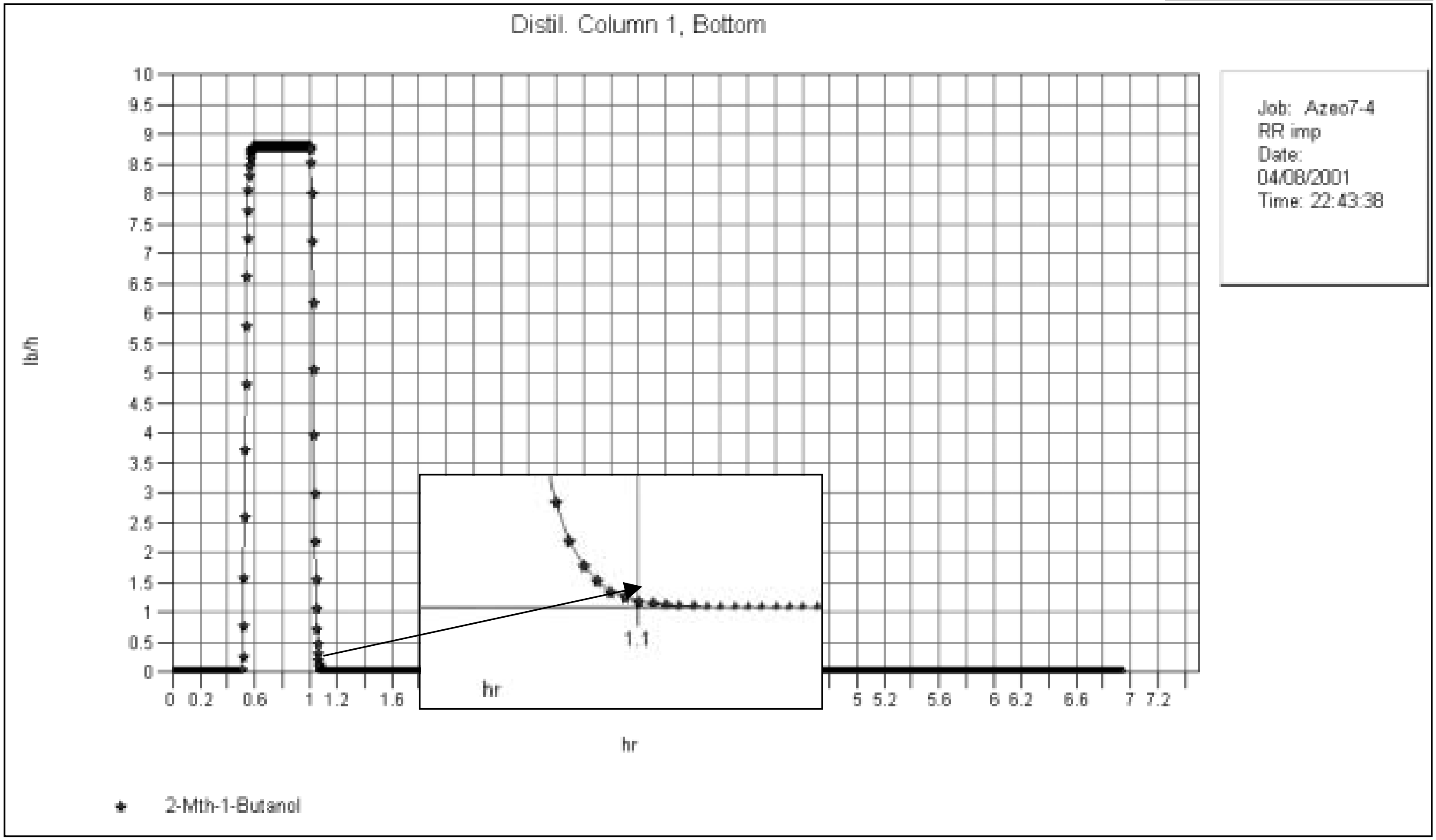


Effect of cooling water temperature change

Effect of feed change on column pressure control:



Response to feed impurities:

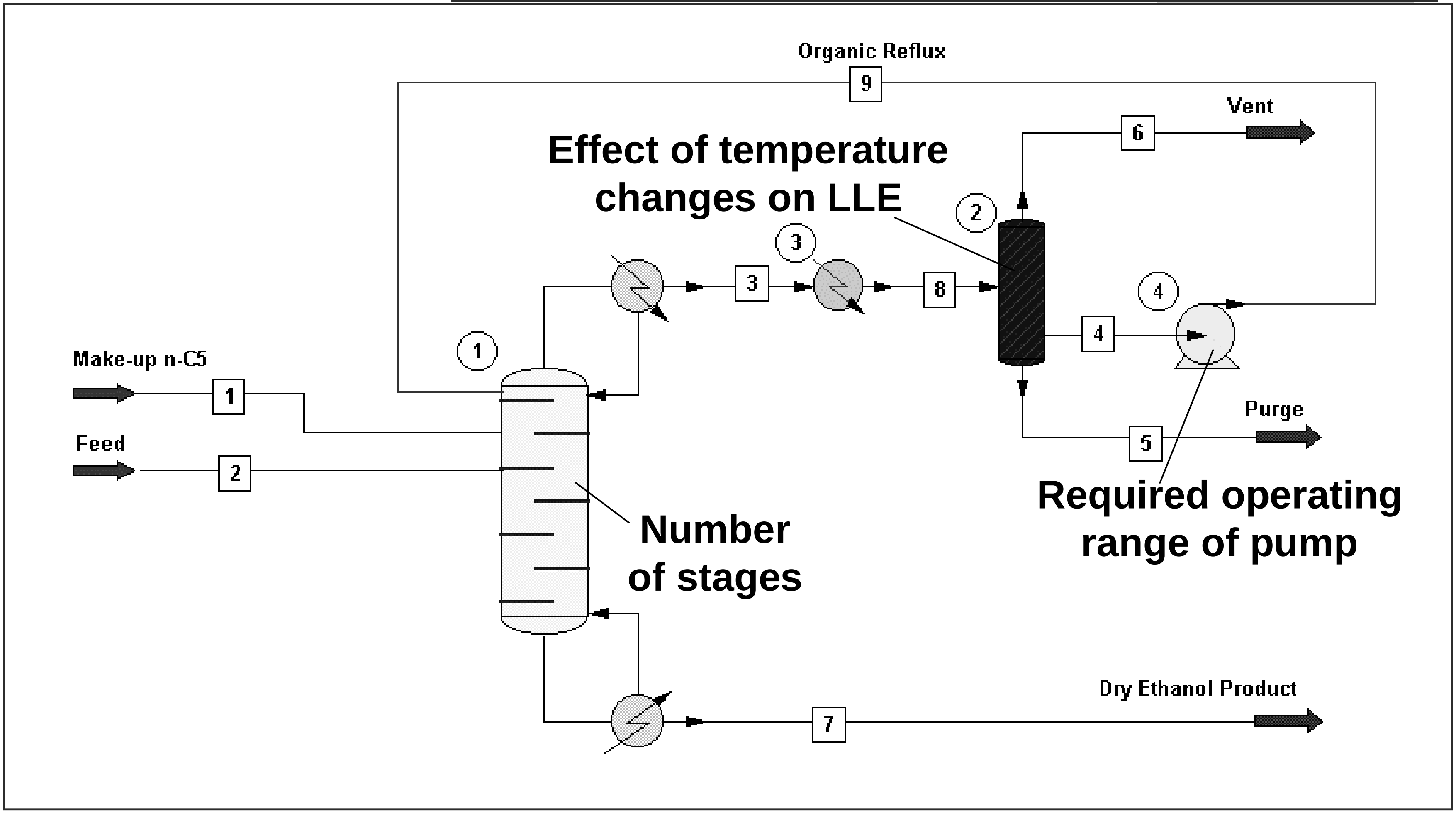


Equipment Which Can Be Included:

- Distillation
- Reactors (CSTR’s, PFR’s special models)
- Heat Exchangers
- Prime movers = pumps, compressors, etc.
- Pipes
- Valves
- Vessels and Tanks
- PID Controllers

So What?

Benefits of “reality” simulations:



Some final notes

Mass Transfer in Distillation Calculations (cont.)

TWO TYPES OF METHODS:

1) **Methods of the first type begin with the mass and heat balances of an differential element of the packing or of the two-phase layer on the plate.**

2) **The other group of methods of simulation for multicomponent separation is the non-equilibrium stage model pioneered by Krishnamurty and Taylor.**

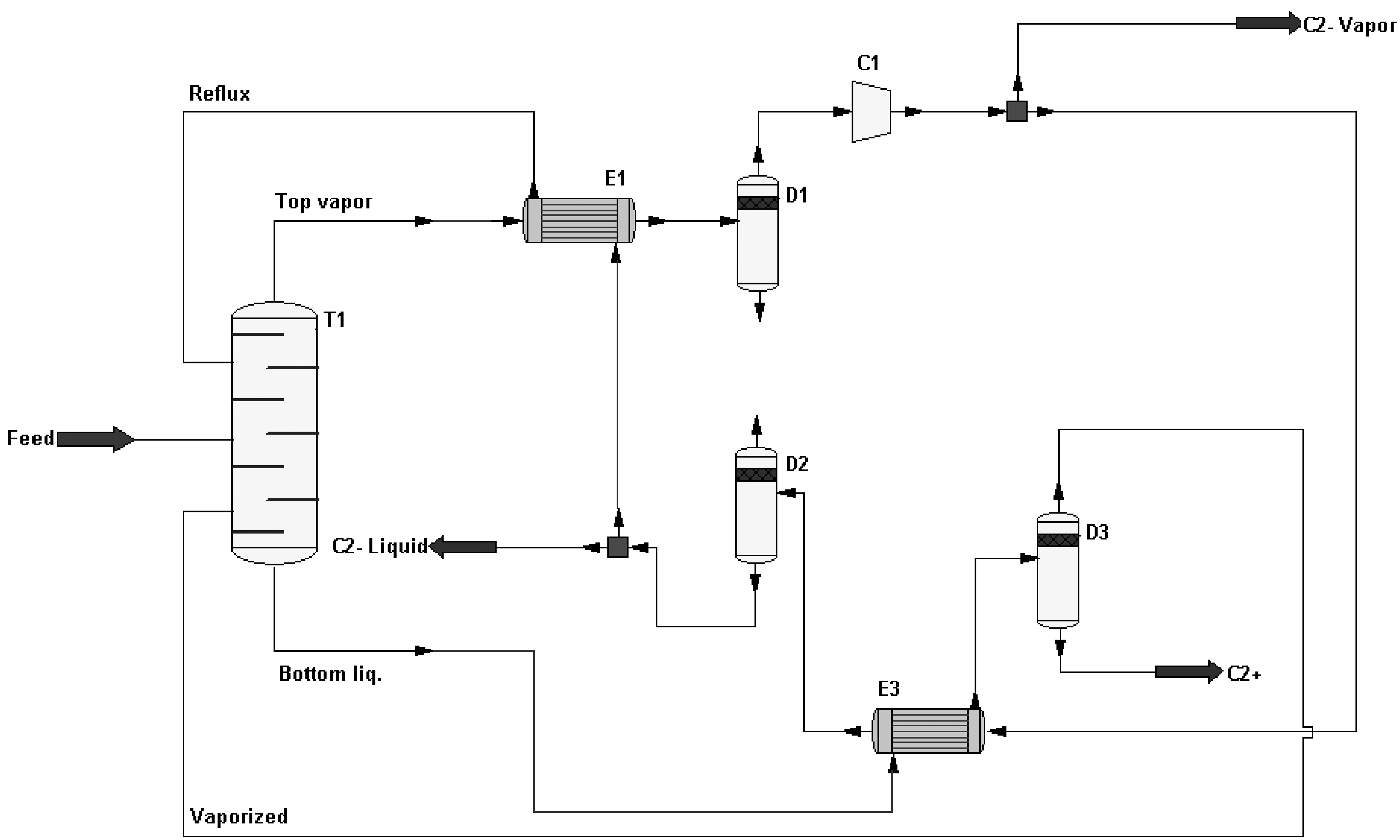
Both types of methods give basically the same results. At present, the latter model is the more accepted approach.

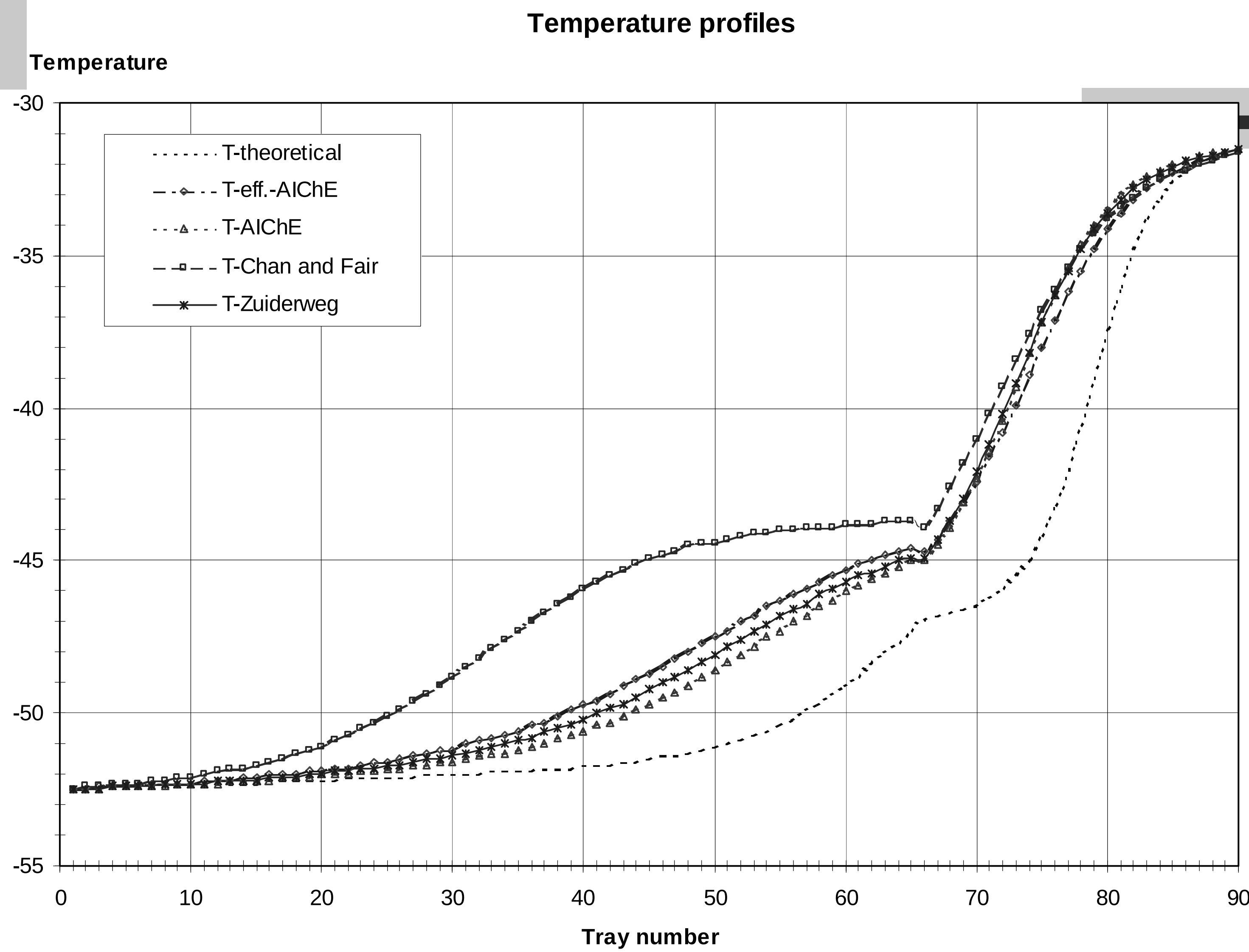
Mass Transfer in Distillation Calculations (cont.)

In this presentation some examples of experimentally verified rated based distillations are presented. The chosen test systems cover a range of components which exhibiting various degrees of differences in chemical structure and in the binary diffusivities and/or enthalpies of vaporization.

- **Ethanol/water/n-pentane**
- **Ethane/Ethylene**
- **Formaldehyde/water/methanol**
- **HCl/water/air**

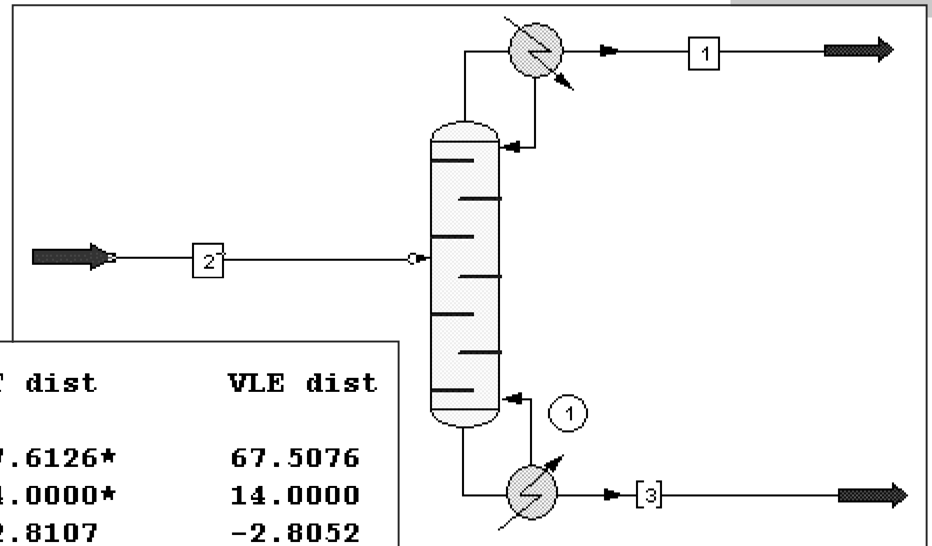
Ethane - Ethylene splitter Technology





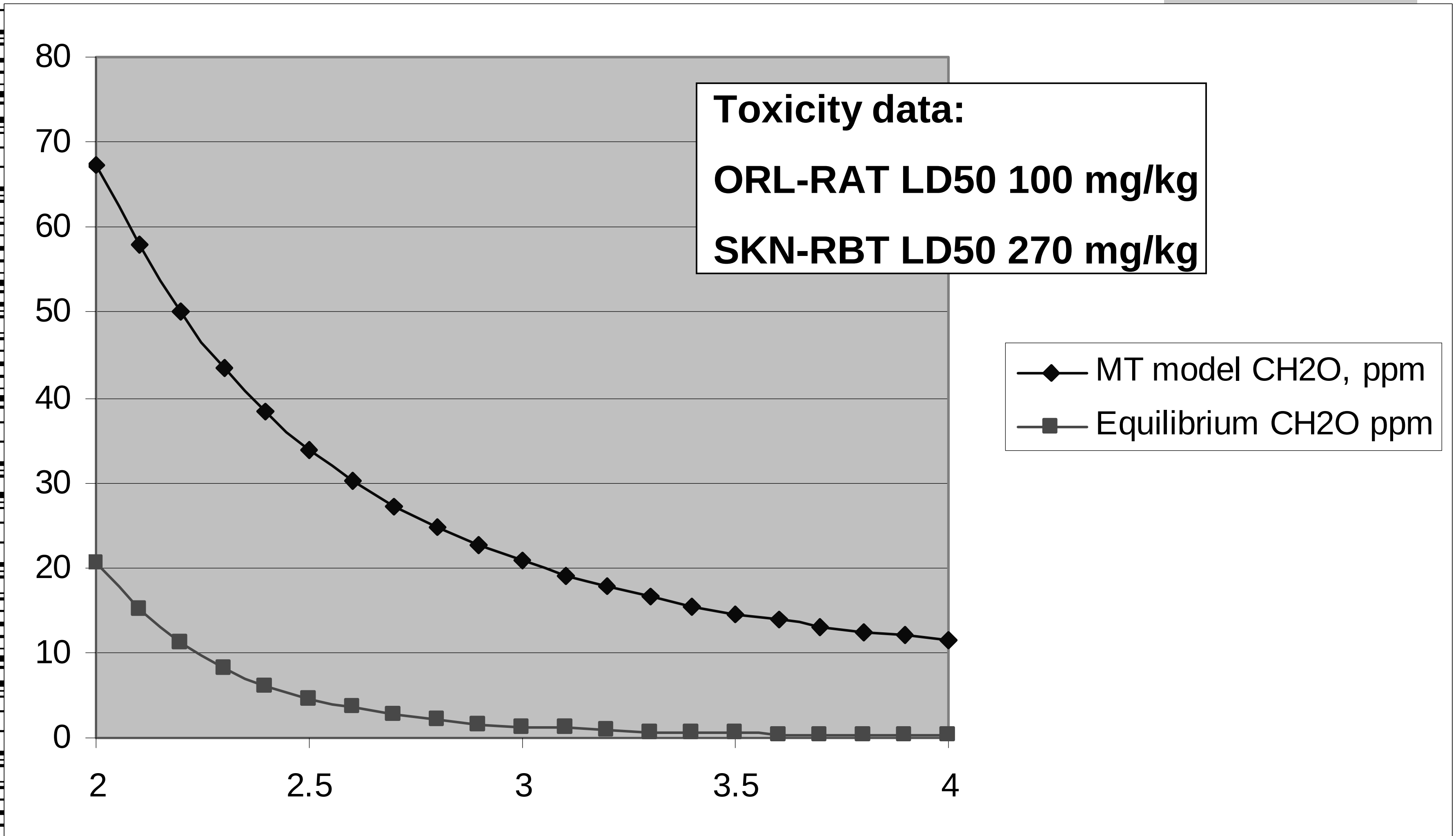
Temperature profiles
Temperature
-30
-35
-40
-45
-50
-55
T-theoretical
T-eff.-AIChE
T-AIChE
T-Chan and Fair
T-Zuiderweg
0
10
20
30
40
50
60
70
80
90
Tray number

Formaldehyde/Water/Methanol:



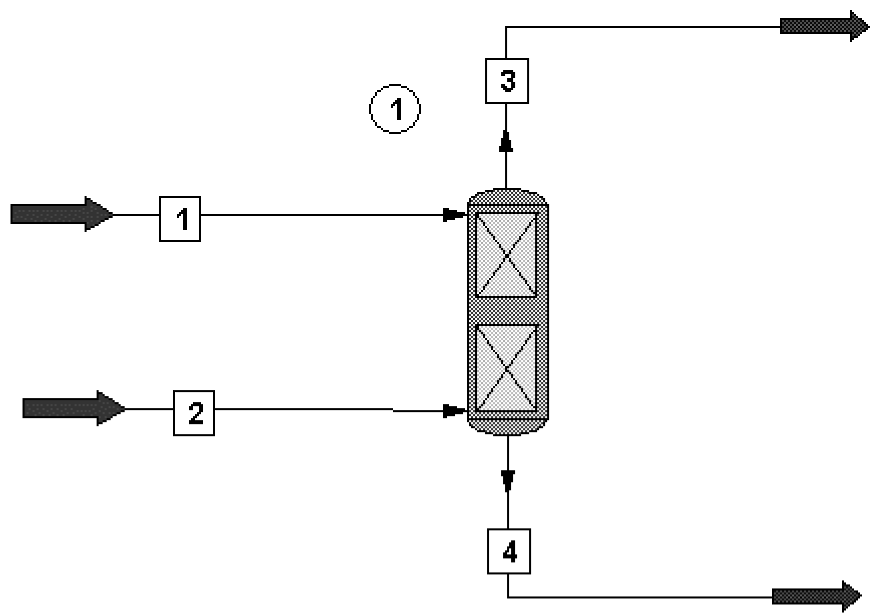
Stream No.	MT dist	VLE dist
Stream Name		
Temp C	67.6126*	67.5076
Pres psia	14.0000*	14.0000
Enth MMBtu/h	-2.8107	-2.8052
Vapor mole fraction	0.00000	0.00000
Total lbmol/h	24.7424	24.7161
Total lb/h	874.3914	875.7383
Total std L gpm	2.0923	2.0970
Total std V scfh	8883.31	8873.87
Component mass fractions		
Water	0.092872	0.089523
Methanol	0.678298	0.682064
Formaldehyde	0.000100	0.000034
N-Butyl Acetate	0.228730	0.228379
Phenol	0.000000	0.000000

Formaldehyde/Water/Methanol:



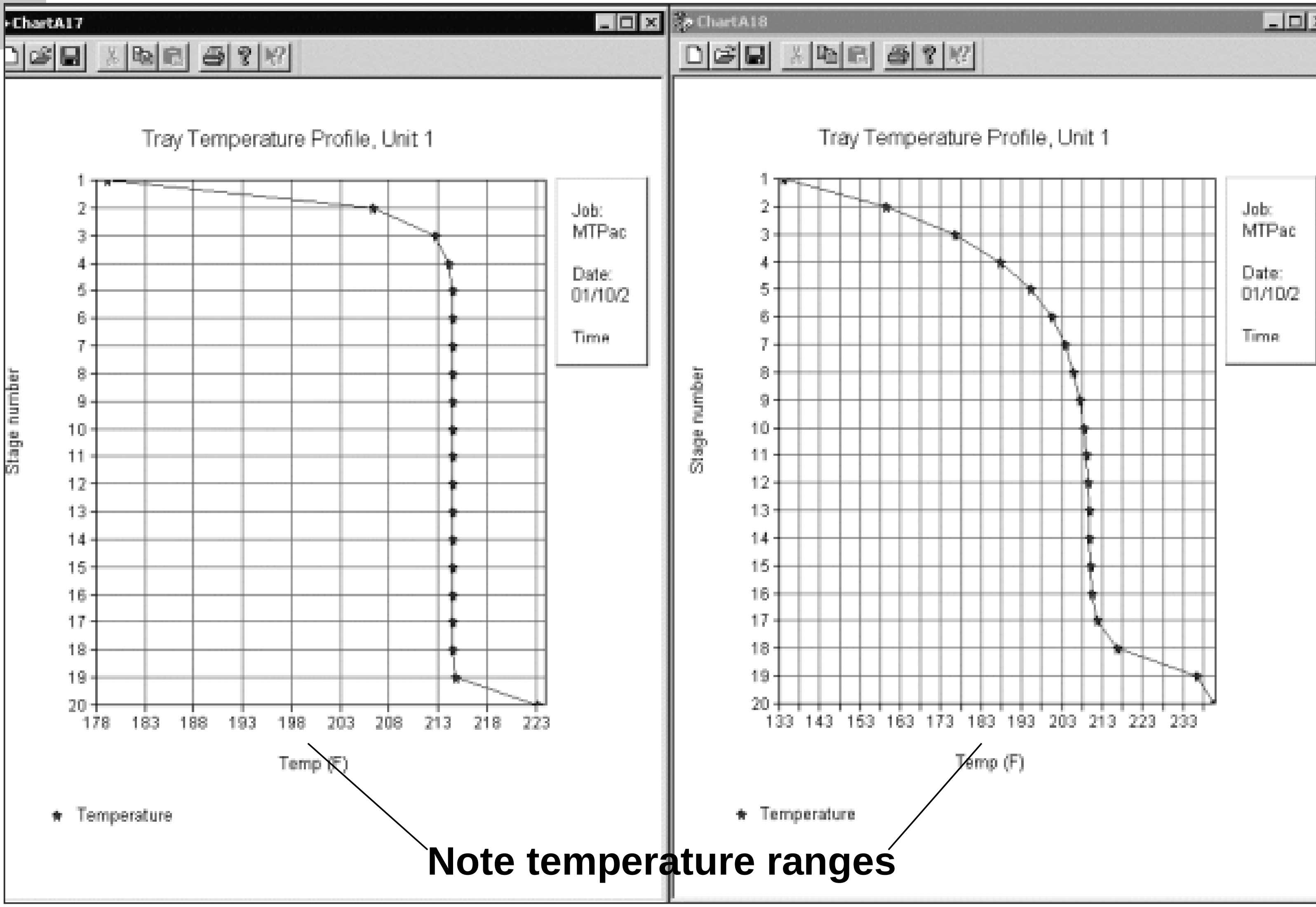
HCl Scrubbing:

Packed column mass transfer



Stream No.	1	2	3	4
Name				
- - Overall - -				
Molar flow lbmol/hr	251.0000	130.0000	116.6215	264.3785
Mass flow lb/hr	4540.2109	3974.9302	3180.4668	5334.6743
Temp F	100.0000	100.0000	179.0061	223.1575
Pres psia	50.0000	50.0000	50.0000	50.0000
Vapor mole fraction	0.0000	1.000	1.000	0.0000
Enth MMBtu/hr	-30.710	-1.1717	-1.6467	-30.235
Actual vol ft3/hr	73.4892	15572.6572	15957.3486	111.7490
Std liq ft3/hr	72.8439	74.1990	58.3214	88.7215
Std vap 60F scfh	95249.1328	49332.2227	44255.3789	100325.9922

HCl Scrubbing:



Note temperature ranges

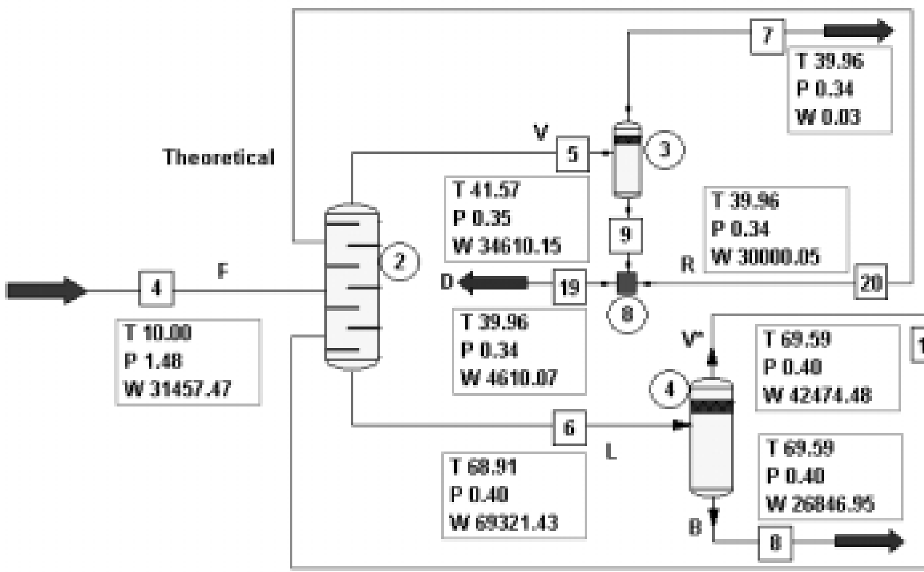
Mass Transfer in Distillation Calculations (cont.)

The rate-based approach is recommended for modeling of the following operations:

- **Packed columns**
- **Mixtures which exhibit strongly non-ideal behavior**
- **Reactive distillation**
- **Any column with profiles of rapidly changing slope**

Thank You …

End

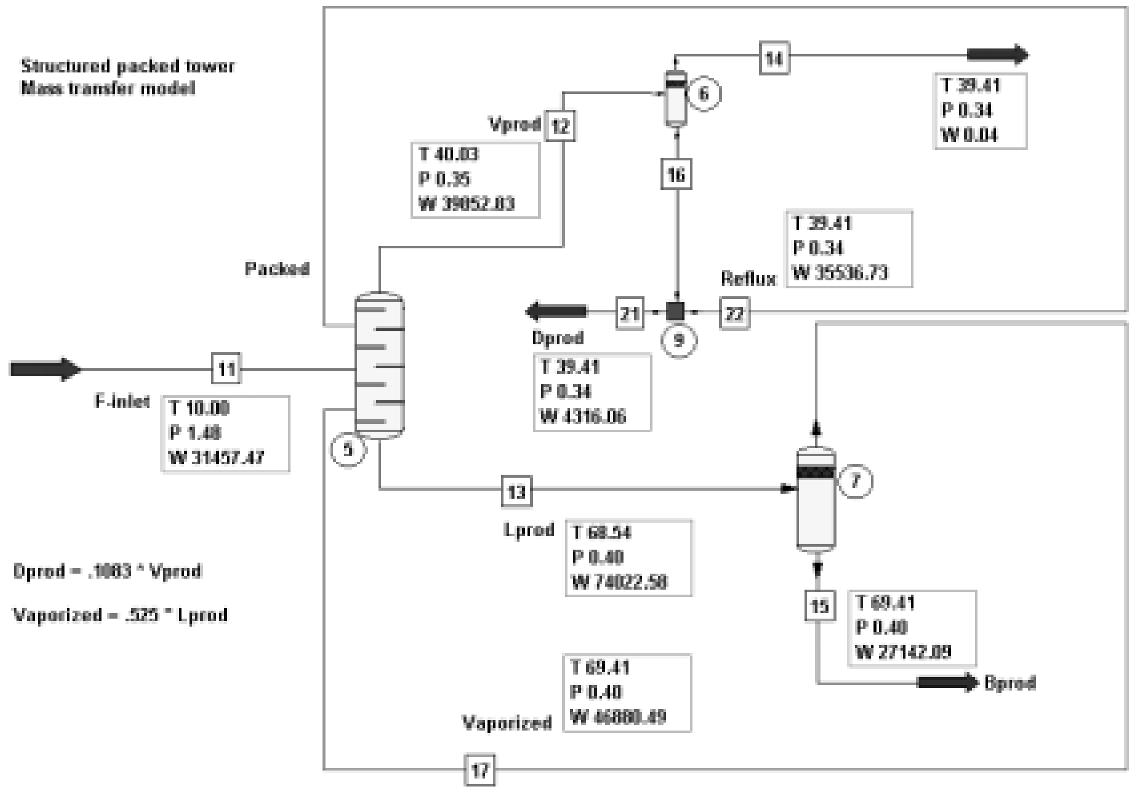


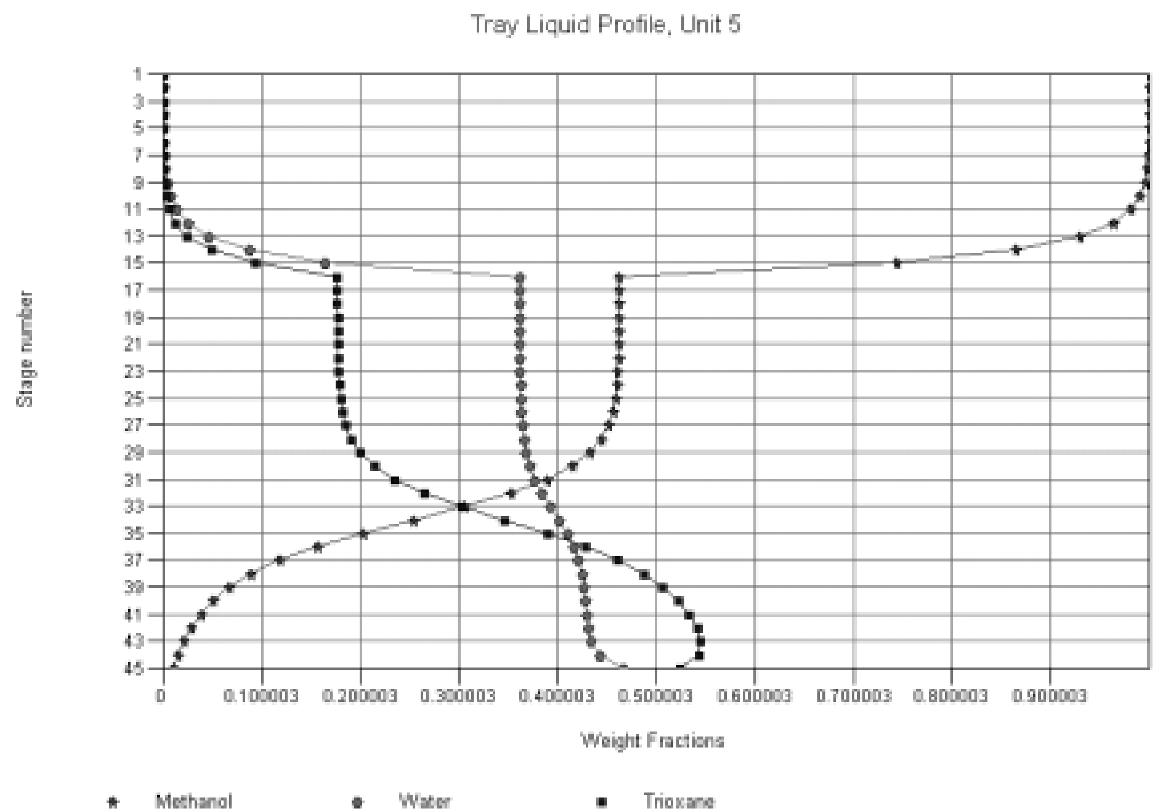
V=R+D
Rr=R/D
Vfr=D/V=1/(Rr+1)

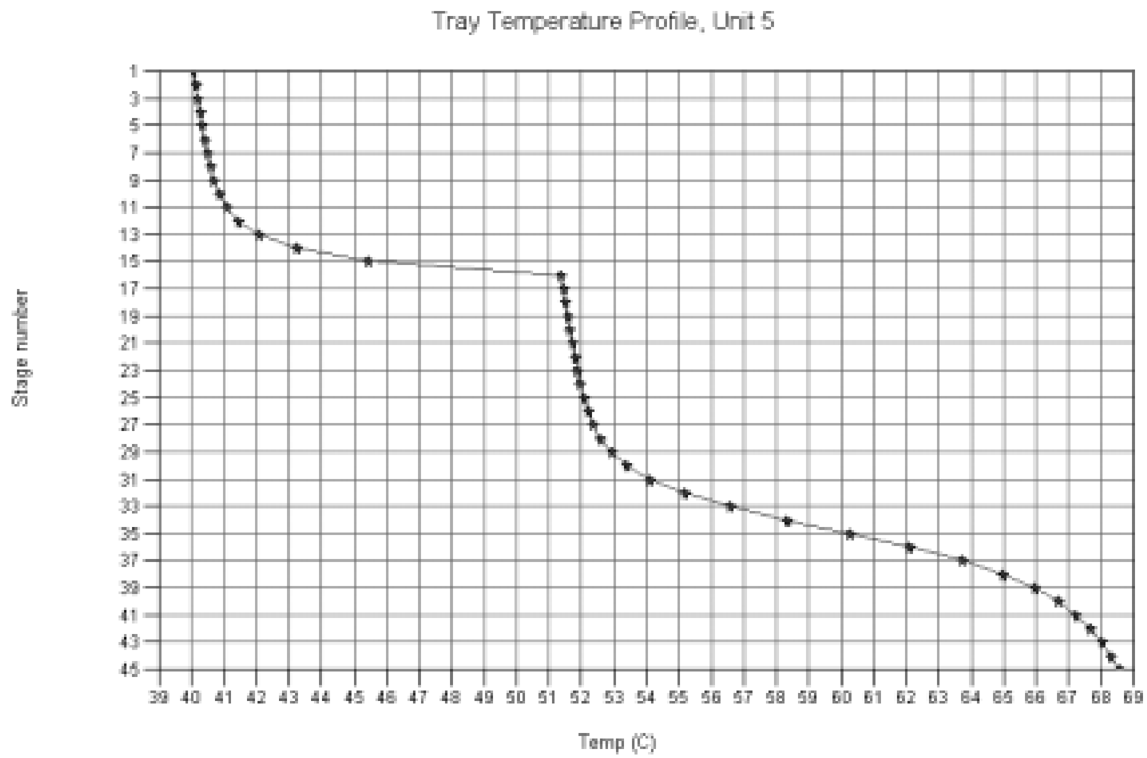
Vfr = .1332
see divider setting

L=B+V*
Vr=V*/B
Vfr=V*/L=Vr/(Vr+1)

Vfr = .5
see flash setting


Structured packed tower
Mass transfer model
Vprod
12
T 40.03
P 0.35
W 39052.03
14
6
T 39.41
P 0.34
W 0.04
16
T 39.41
P 0.34
W 35536.73
Reflux
Packed
21
9
22
Dprod
T 39.41
P 0.34
W 4316.06
11
F-inlet
T 10.00
P 1.40
W 31457.47
5
13
7
Lprod
T 68.54
P 0.40
W 74022.58
15
T 69.41
P 0.40
W 27142.09
Bprod
Dprod = .1083 * Vprod
Vaporized = .525 * Lprod
T 69.41
P 0.40
W 46880.49
Vaporized
17


Tray Liquid Profile, Unit 5
Stage number
Weight Fractions
0
0.100003
0.200003
0.300003
0.400003
0.500003
0.600003
0.700003
0.800003
0.900003
1
3
5
7
9
11
13
15
17
19
21
23
25
27
29
31
33
35
37
39
41
43
45
Methanol
Water
Trioxane



Tray Temperature Profile, Unit 5
Stage number
Temp (C)
1
3
5
7
9
11
13
15
17
19
21
23
25
27
29
31
33
35
37
39
41
43
45
39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69