Rate Based Distillation Simulation of FRI Test for #2 Nutter Ring Using ChemSep

2012 AIChE Spring Meeting - Houston

Ross Taylor - Clarkson University
Attilio J. Praderio - ConocoPhillips - LNG Technology

This Presentation:

Provides an example of the application of Rate-Based Simulation of an industrial scale column.

while avoiding, as much as possible,

theoretical treatments* [that] *often make formidable reading for the process engineer and it is not easy to pick out a design procedure from the information provided. M.J. Lockett, "Distillation Tray Fundamentals"

Distillation Column Modeling: Equilibrium ⇔ Rate Based

Some Highlights

Equilibrium Models: simultaneous solution of MESH equations

Material Balance, Equilibrium Ratios, Summation of mole fractions, Heat Balance

Both, Gas and Liquid Phases are at the same temperature

Ideal to Actual Stages via "Efficiencies": Point => Tray => Section => Column

Rate Base Models: simultaneous heat / mass transfer rates based on Driving Forces

(Transfer Rate /Unit Area) = Flux = (Transfer Coefficient) X (Driving Force)

Individual Temperatures for Gas and Liquid Phases

Individual Separation Efficiencies: Component by Component & Stage by Stage

"Stage Efficiencies" can be back-calculated and applied to Equilibrium Models

Distillation Column Modeling: Equilibrium ⇔ Rate Based

Some Highlights

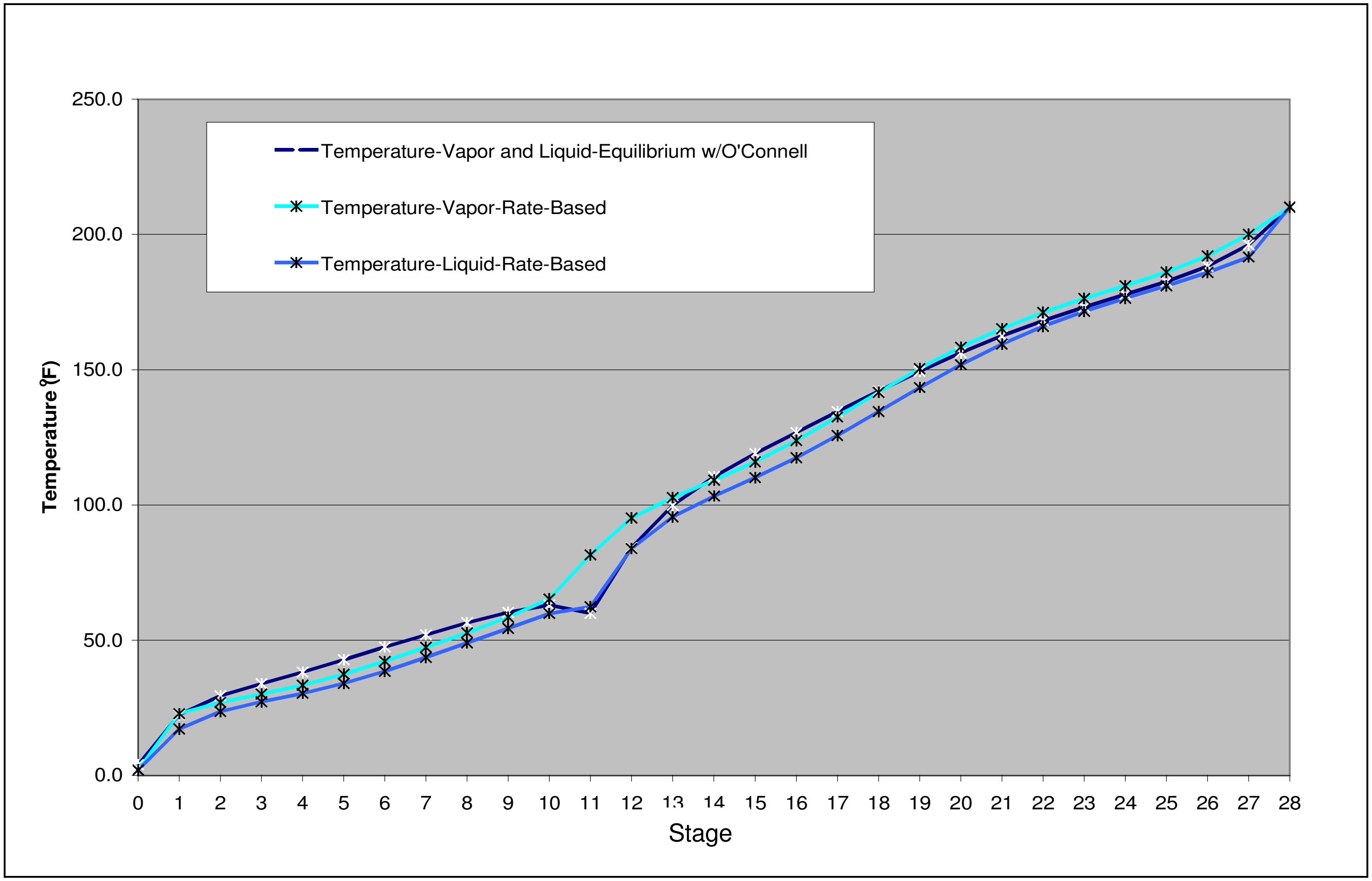
Both Models:

- Results agree within 4% when Rate Base back-calculated efficiencies are incorporated in Equilibrium Models.
- Accuracy depends on selection of proper
  - VLE model (EOS and corresponding BiPs) => Liquid and Vapor Composition
  - Mass Transfer / Flow Pattern model selection
  - Physical Properties estimation (component and mixture)
- Can match field results

Distillation Column Modeling: Equilibrium ⬄ Rate Based

Some Highlights => Temperature Profiles

Different Vapor and Liquid Temperatures (RB) vs Equal Temperatures (EQM)
Apparent Small Differences in the Temperature Profiles, BUT..

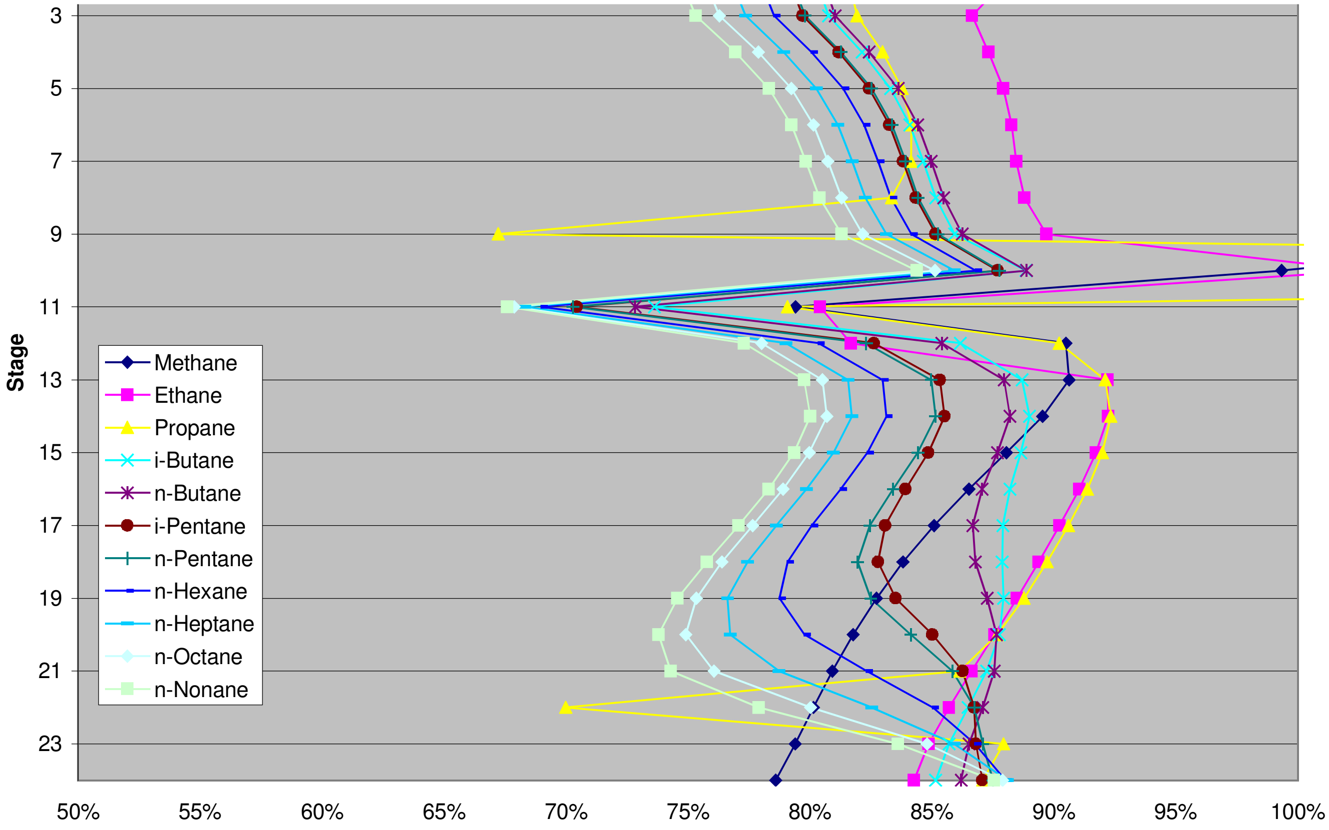


Distillation Column Modeling: Equilibrium ⇔ Rate Base,

Some Highlights => Separation Efficiencies

… In Multicomponent Mixtures,

Separation Efficiencies are different for every component at each stage



And despite Individual stage efficiency can be back-calculated and used in Equilibrium Models….

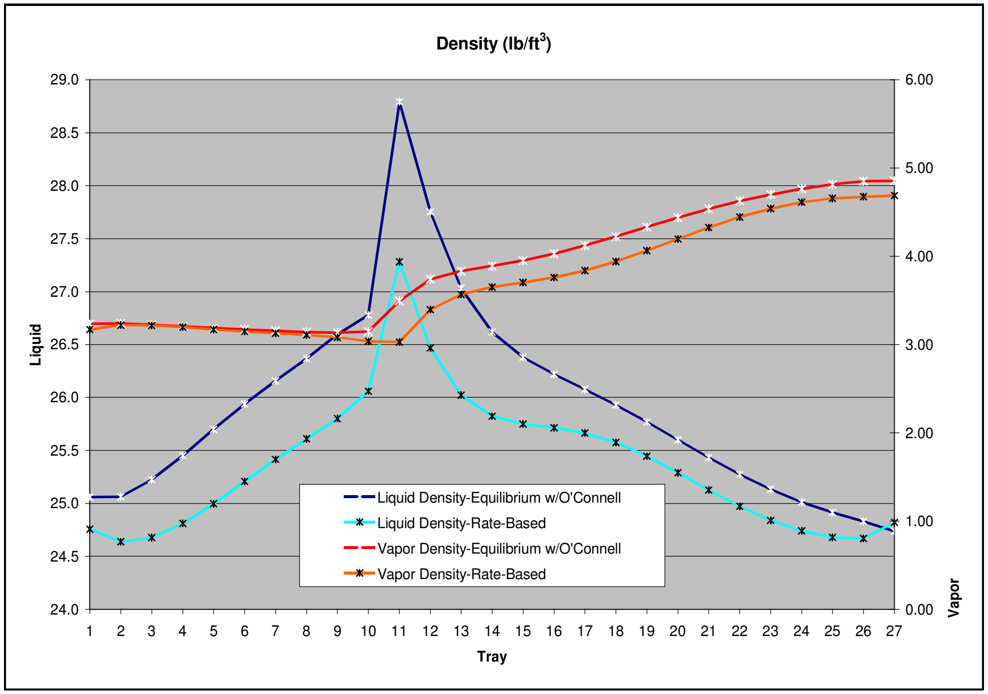
Distillation Column Modeling: Equilibrium ⇔ Rate Base,

Some Highlights => Physical Props Estimation and Hydraulics Performance

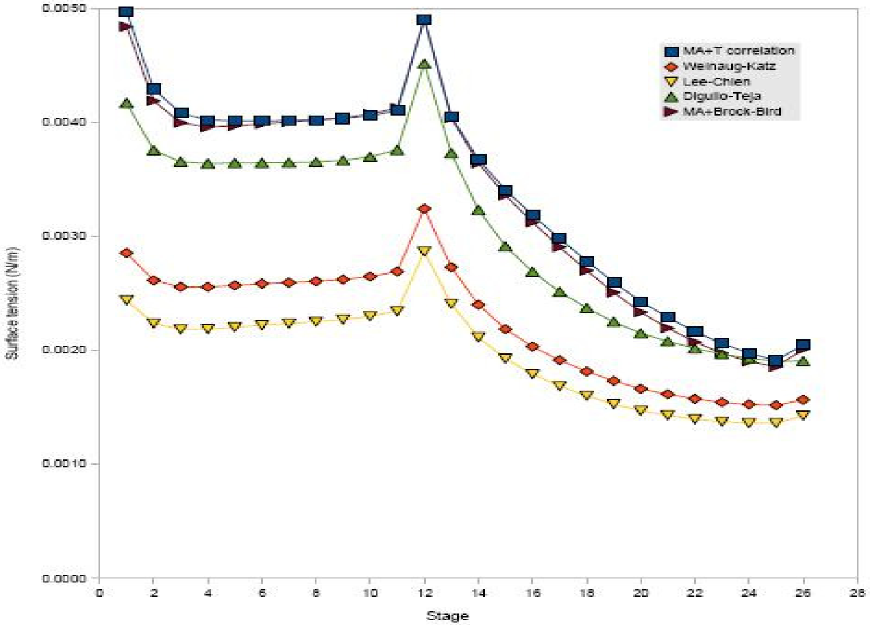
The compositional differences effect the estimation of the physical properties related to Tower Capacity :

- Approach to flood (ρ,σ)

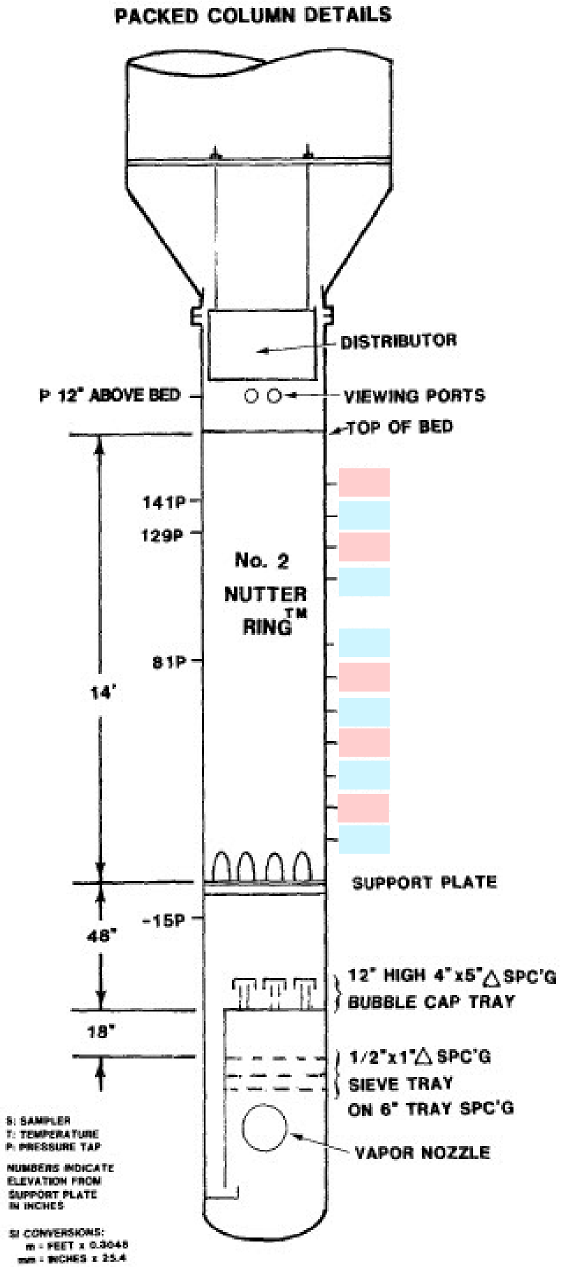
- System Limit (ρ,σ)



Surface Tension = f (liquid density – gas density)[4]



FRI Test Column Arrangement for the Nutter Ring #2



Run Type		Tot Ref
Reboiler Duty	(MMBtu/hr)	5.84
Condenser Duty	(MM Btu/hr)	5.87
Reflux	(M lbs/hr)	34.51
Feed	(M lbs/hr)	46.75
Feeed Location		BTM
Tp Pressure	(psia)	24.0

Temperatures		
Bed Length	F	C
Overhead Va	212.80	100.44
Accumulator	168.90	76.06
Reflux	169.10	76.17
147	214.20	101.22
123	217.20	102.89
75	226.60	108.11
51	229.50	109.72
27	234.20	112.33
Reboiler Vap	238.60	114.78
Reboiler Liqu	239.90	115.50
Feed	235.50	113.06

Concentrations		
Bed Length	Cyclo-C6	n-C7
Overhead Vapor		
Accumulator		
Reflux	0.8683	0.1317
135	0.7596	0.2404
111	0.6458	0.3542
87	0.5192	0.4808
63	0.3957	0.6043
39	0.2553	0.7447
15	0.1753	0.8247
Bottoms	0.0789	0.9211

ChemSep Set Up: Selection of Input Data and Checking Points

Run Type		Tot Ref
Reboiler Duty	(MMBtu/hr)	5.84
Condenser Duty	(MM Btu/hr)	5.87
Reflux	(M lbs/hr)	34.51
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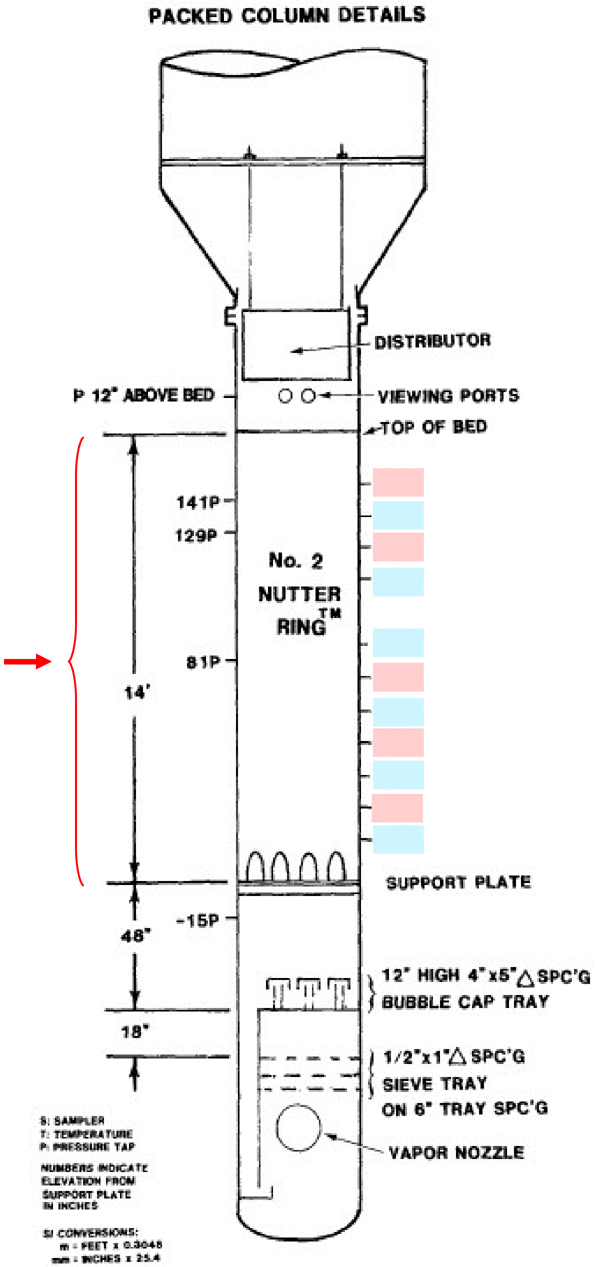
Tp Pressure	(psia)	24.0

-> Input to Simulation
<- Checking Parameter

14 feet of bed
Simulated as 42 segments of 4 inches each segment



Temperatures

Bed Length	F	C
Overhead Va	212.80	100.44
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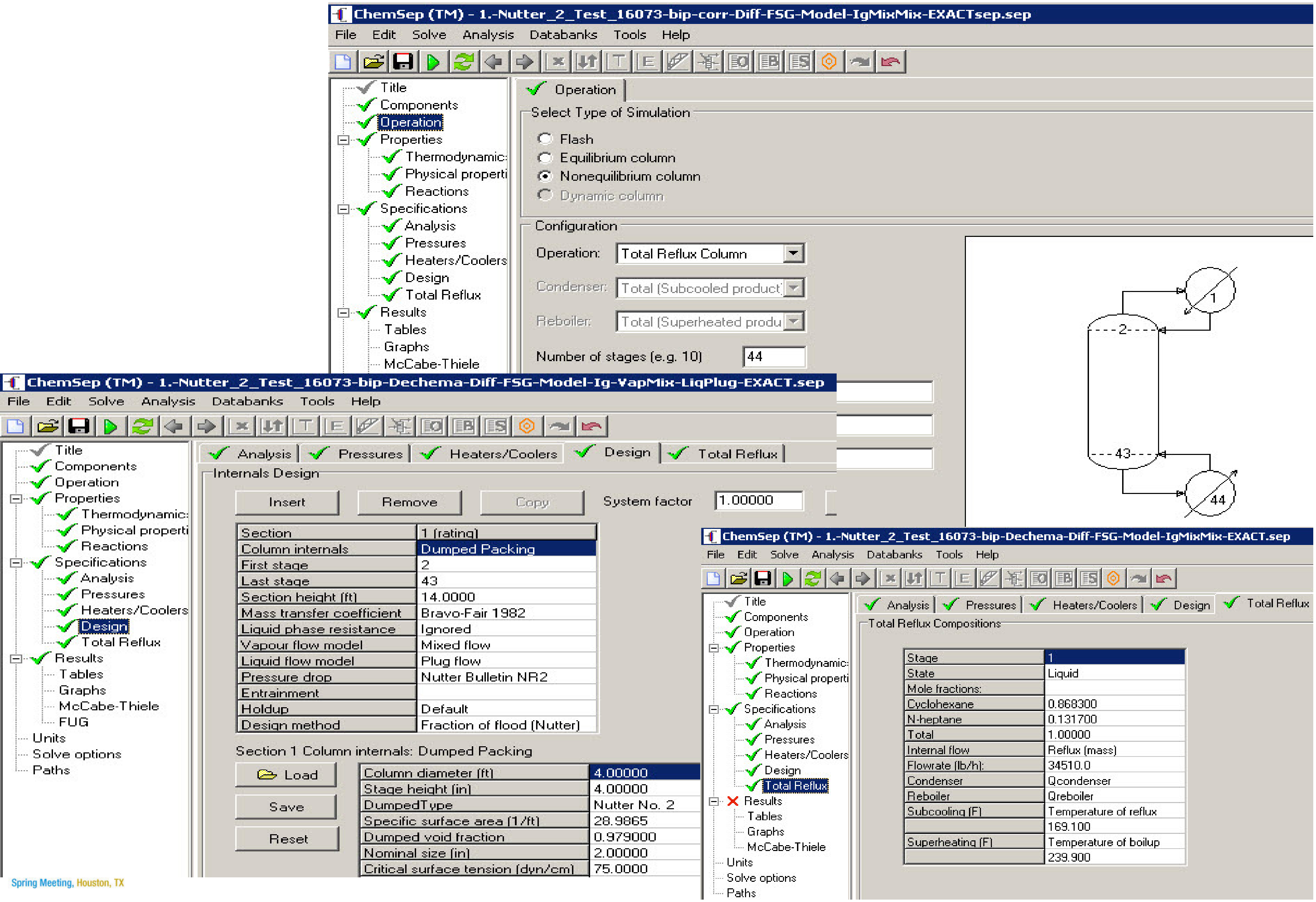
ChemSep - Set Up: Filling in the Data (1/2)



ChemSep (TM) - 1.-Nutter_2_Test_16073-bip-corr-Diff-FSG-Model-IgMixMix-EXACTsep.sep

Operation

Select Type of Simulation

○ Flash
○ Equilibrium column
● Nonequilibrium column
○ Dynamic column

Configuration

Operation: Total Reflux Column
Condenser: Total (Subcooled product)
Reboiler: Total (Superheated produ
Number of stages (e.g. 10) 44

ChemSep (TM) - 1.-Nutter_2_Test_16073-bip-Dechema-Diff-FSG-Model-Ig-VapMix-LiqPlug-EXACT.sep

Analysis | Pressures | Heaters/Coolers | Design | Total Reflux

Internals Design

System factor 1.00000

Section	1 (rating)
Column internals	Dumped Packing
First stage	2
Last stage	43
Section height (ft)	14.0000
Mass transfer coefficient	Bravo-Fair 1982
Liquid phase resistance	Ignored
Vapour flow model	Mixed flow
Liquid flow model	Plug flow
Pressure drop	Nutter Bulletin NR2
Entrainment	
Holdup	Default
Design method	Fraction of flood (Nutter)

Section 1 Column internals: Dumped Packing

Column diameter (ft)	4.00000
Stage height (in)	4.00000
DumpedType	Nutter No. 2
Specific surface area (1/ft)	28.9865
Dumped void fraction	0.979000
Nominal size (in)	2.00000
Critical surface tension (dyn/cm)	75.0000

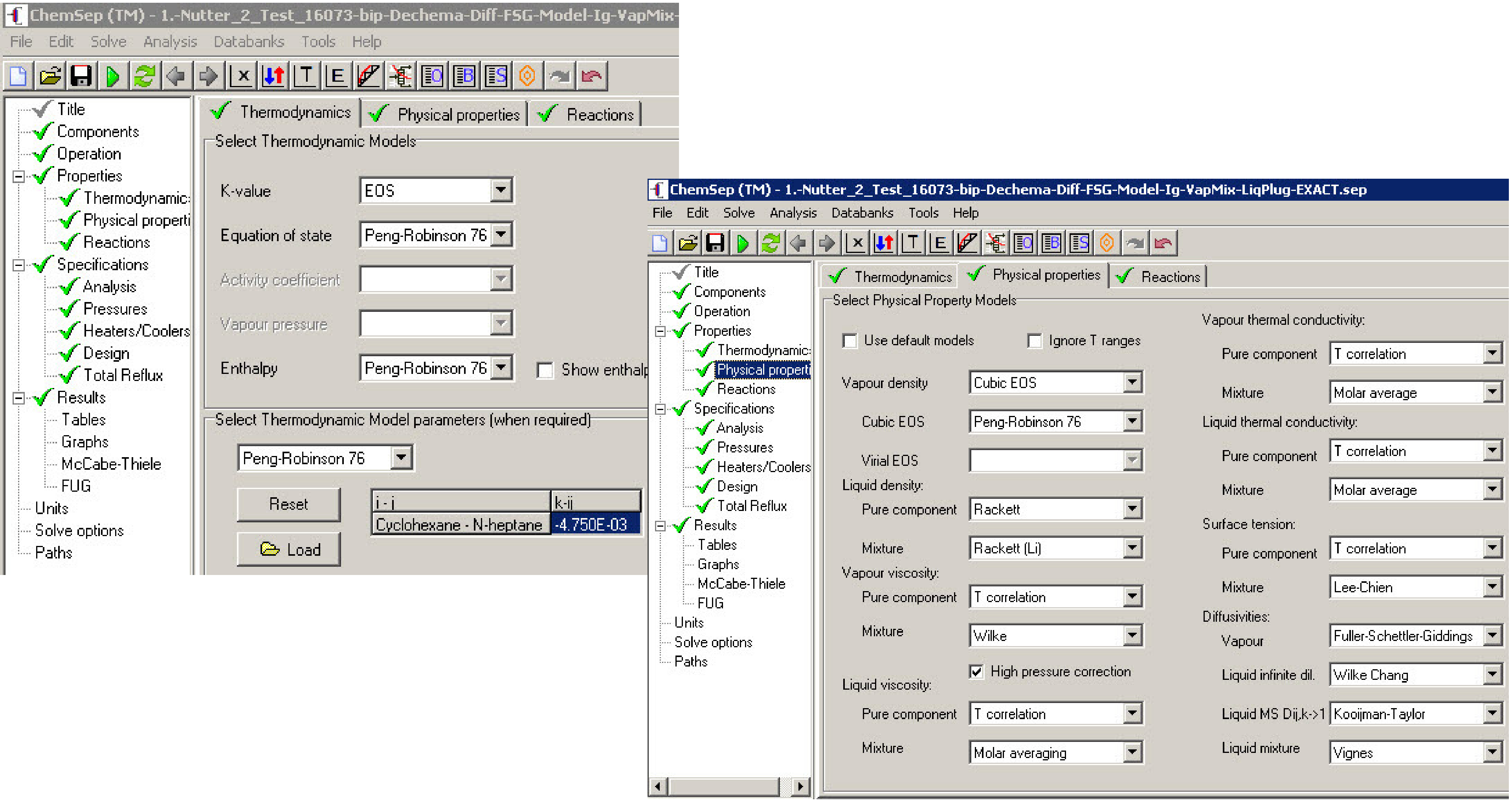
ChemSep (TM) - 1.-Nutter_2_Test_16073-bip-Dechema-Diff-FSG-Model-IgMixMix-EXACT.sep

Analysis | Pressures | Heaters/Coolers | Design | Total Reflux

Total Reflux Compositions

Stage	1
State	Liquid
Mole fractions:	
Cyclohexane	0.868300
N-heptane	0.131700
Total	1.00000
Internal flow	Reflux (mass)
Flowrate (lb/h):	34510.0
Condenser	Qcondenser
Reboiler	Qreboiler
Subcooling (F)	Temperature of reflux
	169.100
Superheating (F)	Temperature of boilup
	239.900

ChemSep - Set Up: Filling in the Data (2/2)



Select Thermodynamic Models

K-value: EOS

Equation of state: Peng-Robinson 76

Activity coefficient:

Vapour pressure:

Enthalpy: Peng-Robinson 76 ☐ Show enthalp

Select Thermodynamic Model parameters (when required)

Peng-Robinson 76

i - j	k-ij
Cyclohexane - N-heptane	-4.750E-03

Select Physical Property Models

☐ Use default models ☐ Ignore T ranges

Vapour density: Cubic EOS

Cubic EOS: Peng-Robinson 76

Virial EOS:

Liquid density:

Pure component: Rackett

Mixture: Rackett (Li)

Vapour viscosity:

Pure component: T correlation

Mixture: Wilke

☑ High pressure correction

Liquid viscosity:

Pure component: T correlation

Mixture: Molar averaging

Vapour thermal conductivity:

Pure component: T correlation

Mixture: Molar average

Liquid thermal conductivity:

Pure component: T correlation

Mixture: Molar average

Surface tension:

Pure component: T correlation

Mixture: Lee-Chien

Diffusivities:

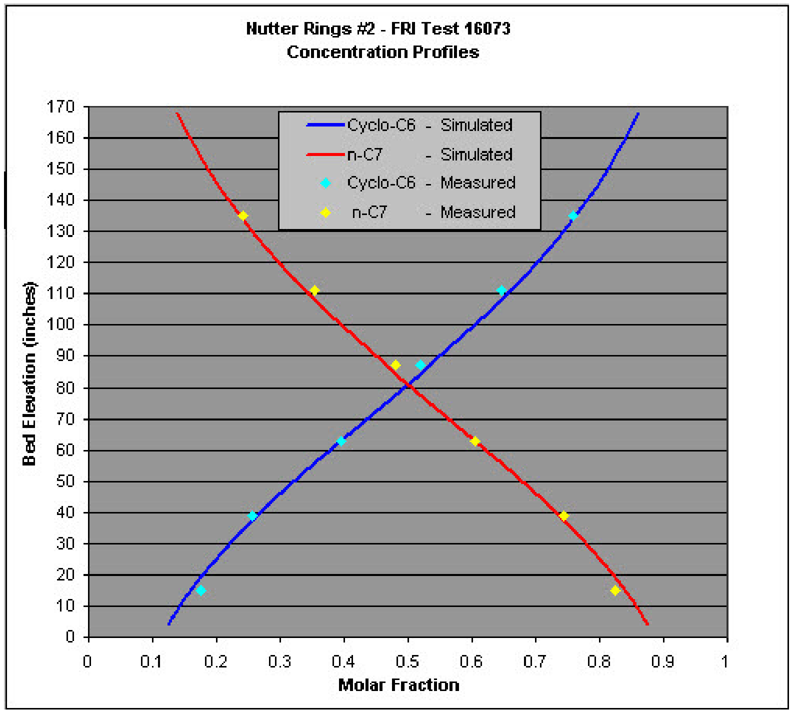
Vapour: Fuller-Schettler-Giddings

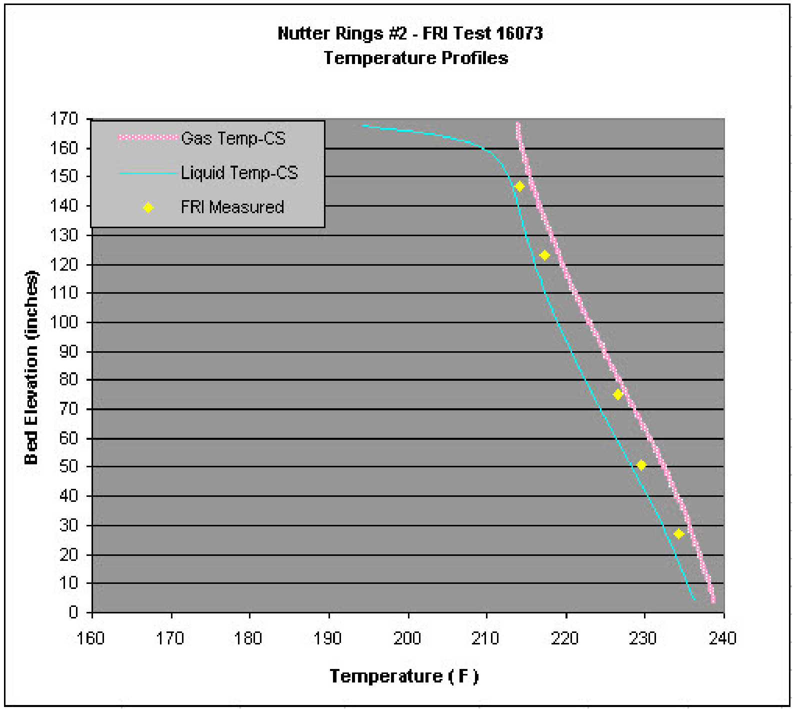
Liquid infinite dil.: Wilke Chang

Liquid MS Dij,k->1: Kooijman-Taylor

Liquid mixture: Vignes

ChemSep - Results: Simulation Results compared to Field Data
Concentration and Temperature Profiles + Heat Duty Required



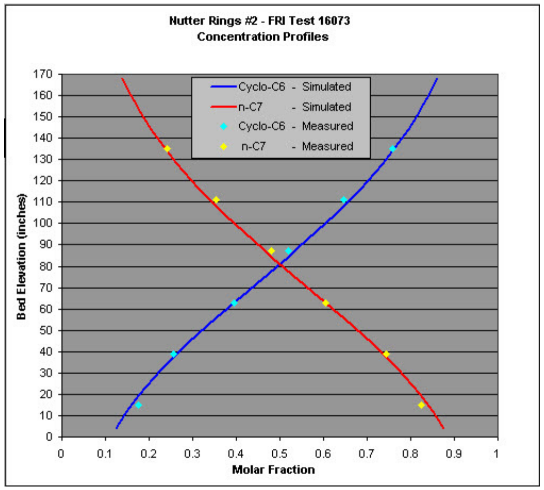


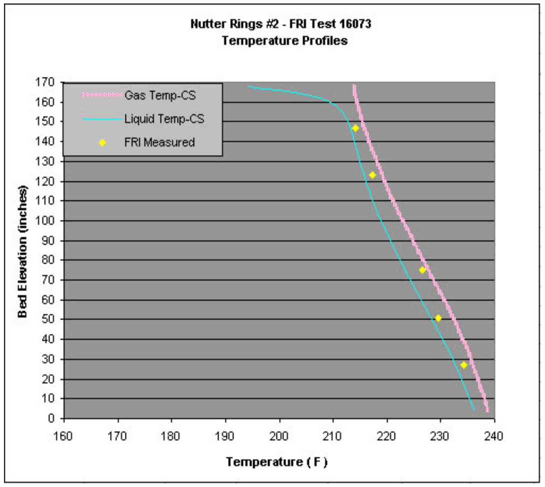
Heat Duties Comparison (MMBTU/hr)

	Measured	Simulated	∠
Condenser	5.87	5.76	1.87%
Reboiler	5.84	5.76	1.37%

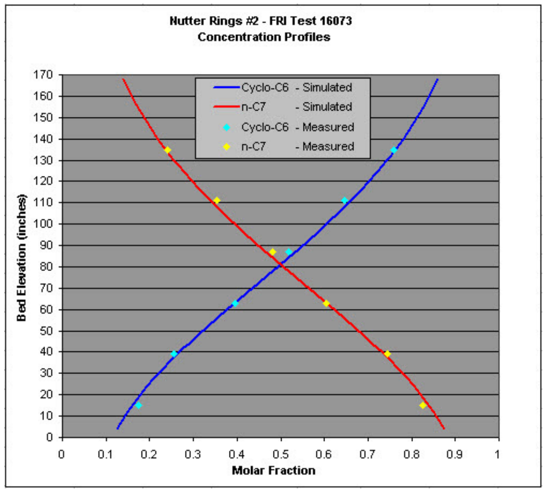
ChemSep - Results: Simulation Results compared to Field Data
Flow Pattern Sensitivity

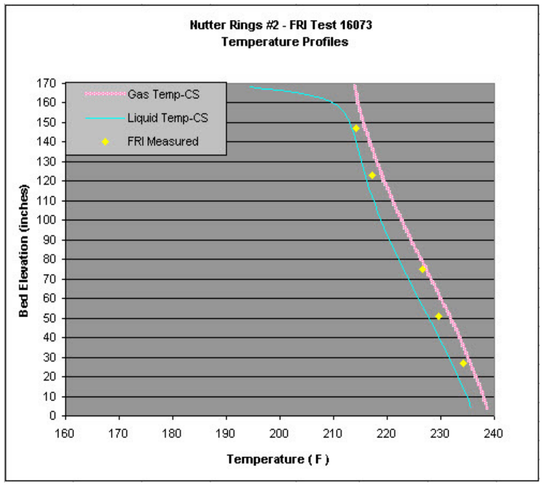
Liquid Res / Vapor / Liquid
Ignored / Mixed / Mixed





Liquid Res / Vapor / Liquid
Included / Plug / Plug





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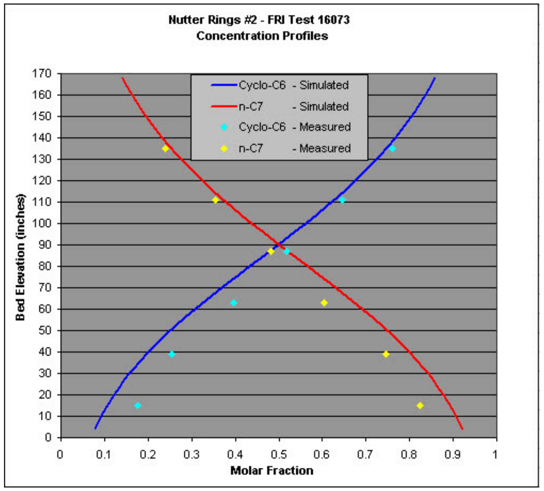

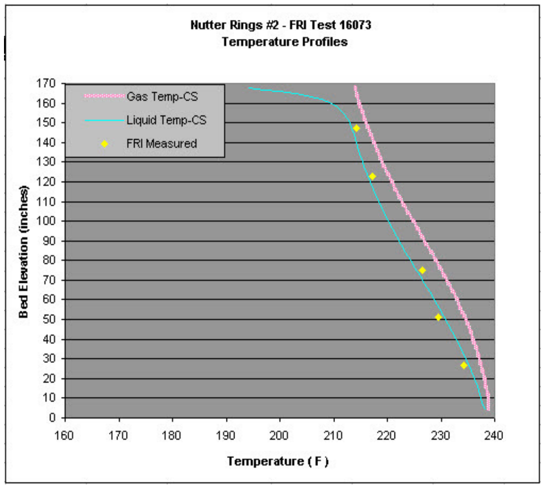

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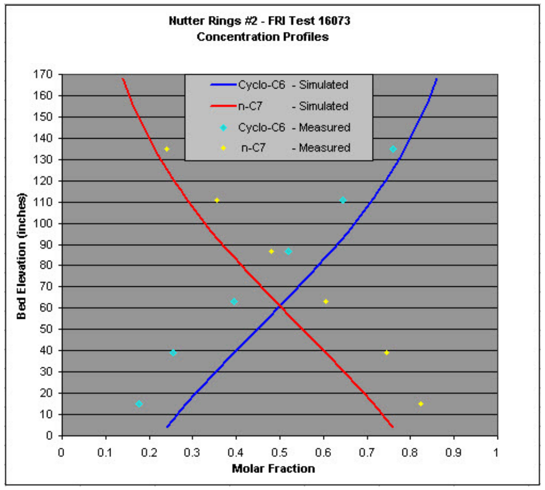

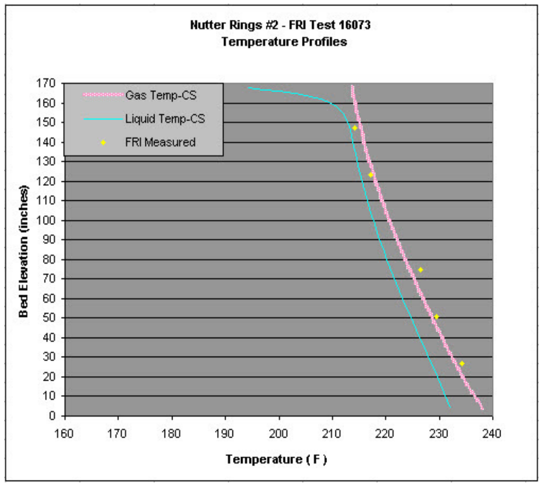

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The Effect of Properties Estimation: EoS and BIP Effects

Component	MW (g/mol)	Composition (mol %)
Nitrogen	28.01	0.246
Carbon Dioxide	44.01	0.143
Methane	16.04	94.045
Ethane	30.07	1.867
Propane	44.10	1.802
i-Butane	58.12	0.356
n-Butane	58.12	0.706
i-Pentane	72.15	0.201
n-Pentane	72.15	0.252
Hexanes:	86.18	0.205
n-Hexane	86.18	0.199
Methylcyclopentane	84.16	0.006
Heptanes +:		
n-Heptane	100.20	0.100
n-Octane	114.23	0.052
n-Nonane	128.26	0.025
Sum	17.88515	100.000

T (K)	P (psia)	P (MPa)
235.99	1396.0	9.625080
247.42	1499.6	10.33937
258.88	1545.8	10.65791
270.14	1542.1	10.63240
289.50	1404.0	9.680238
294.97	1284.4	8.855625
298.64	1162.3	8.013776
303.71	932.15	6.426948
304.52	459.66	3.169244
294.03	188.47	1.299455

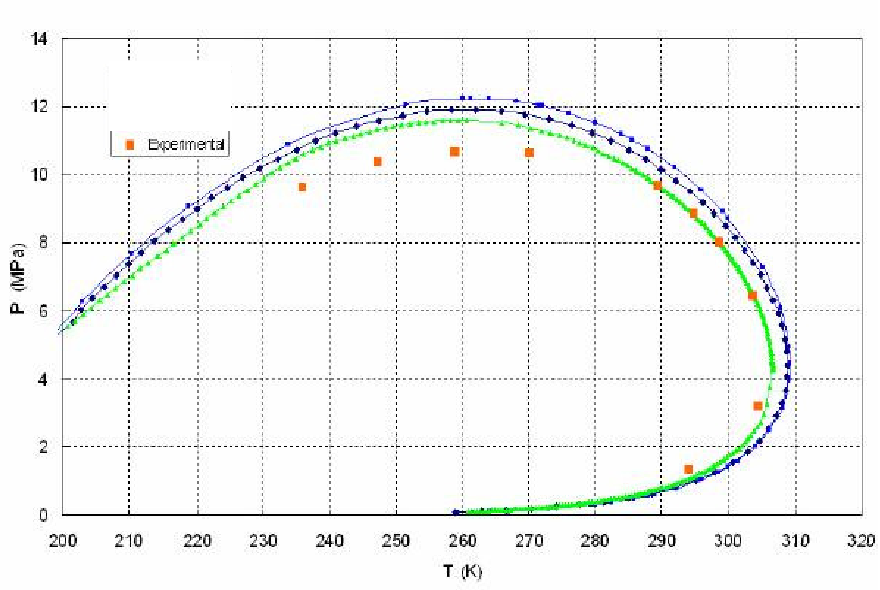


Figure 17. Phase envelope of 94% methane sample comparison with SRK equation.

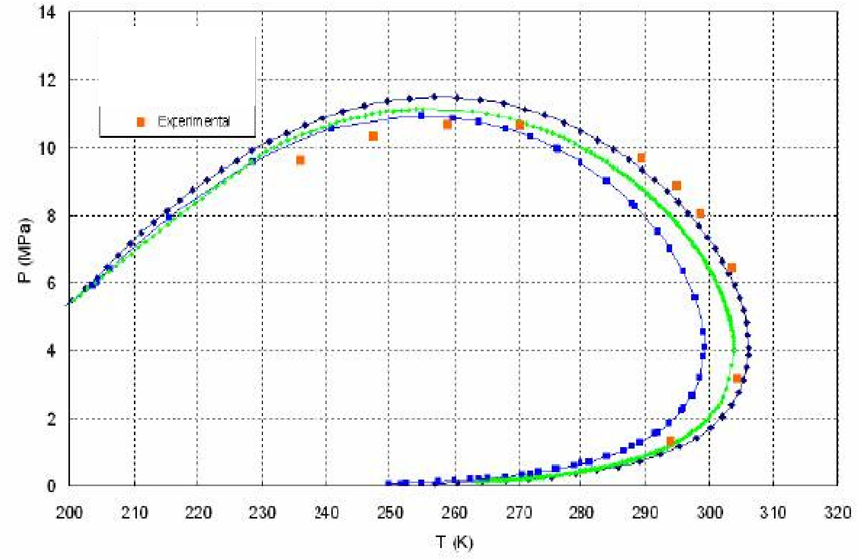
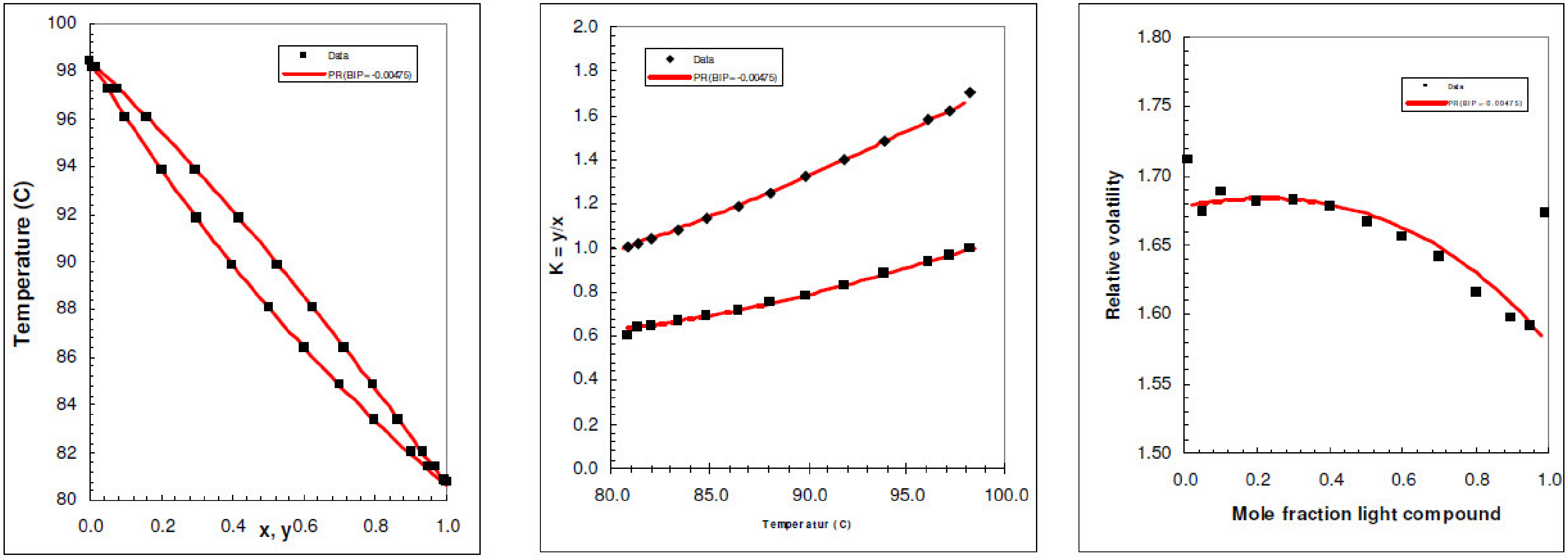


Figure 18. Phase envelope of 94% methane sample comparison with PR equation.

ChemSep Set Up: EOS and BIP verification with VLE data

System: Cyclohexane – n-Heptane at 1 atm



JOURNAL	Ind. Eng. Chem.
VOLUME	51
PAGES	211
YEAR	1959
TITLE	
AUTHORS	C. Black

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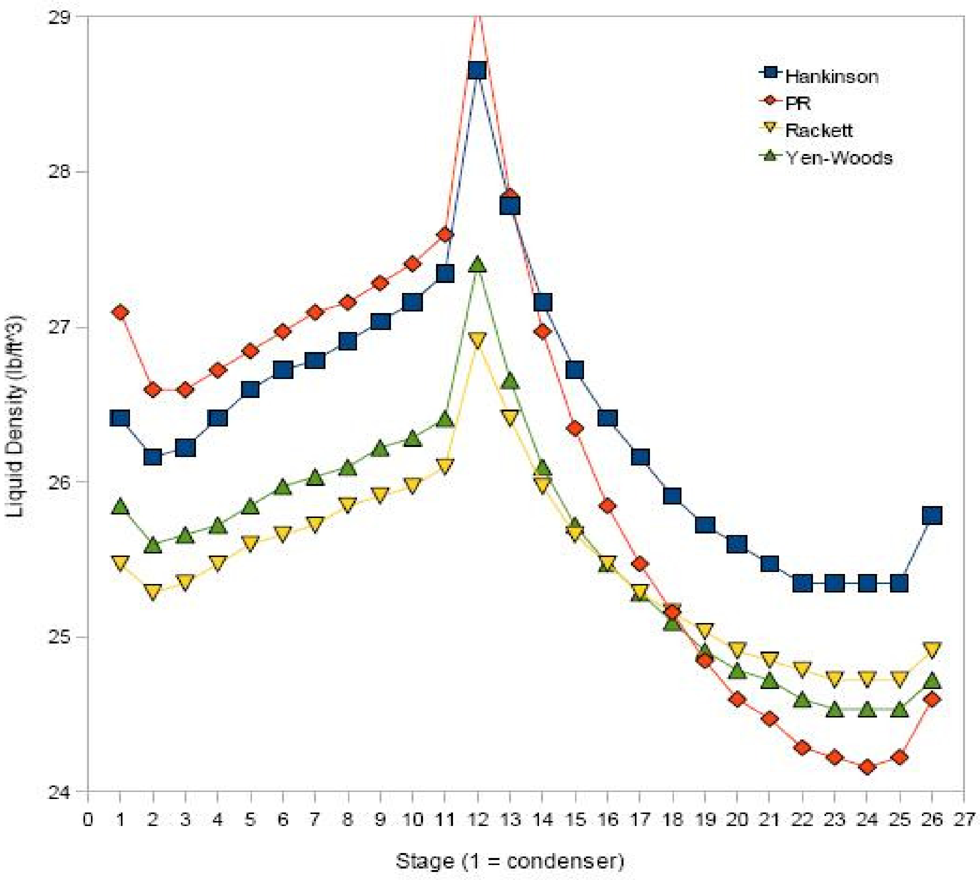
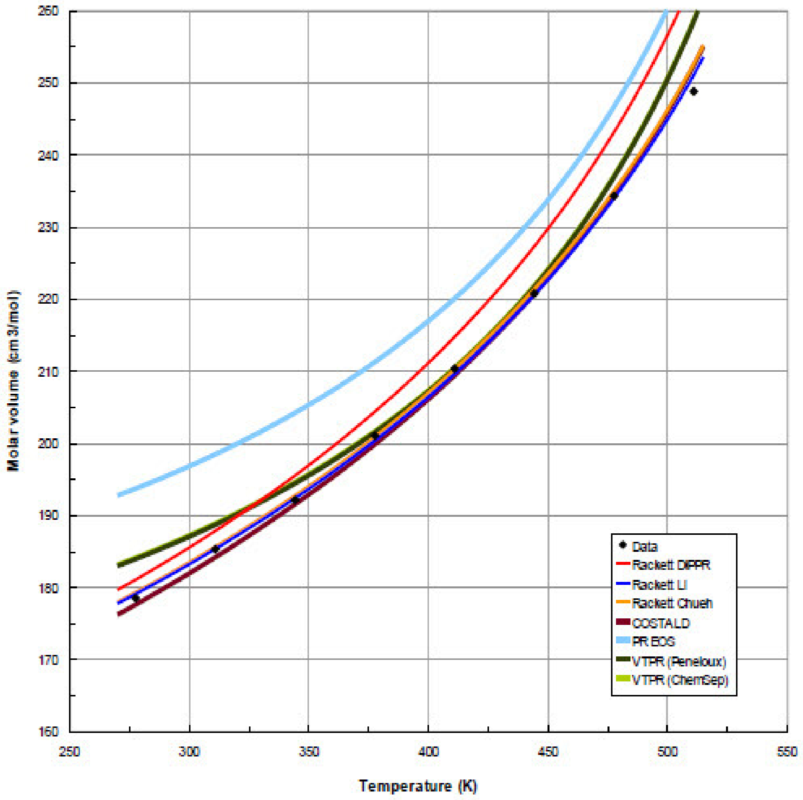
The Effect of Properties Estimation: Liquid Density Estimation

Capacity Loss due to unexpected flooding

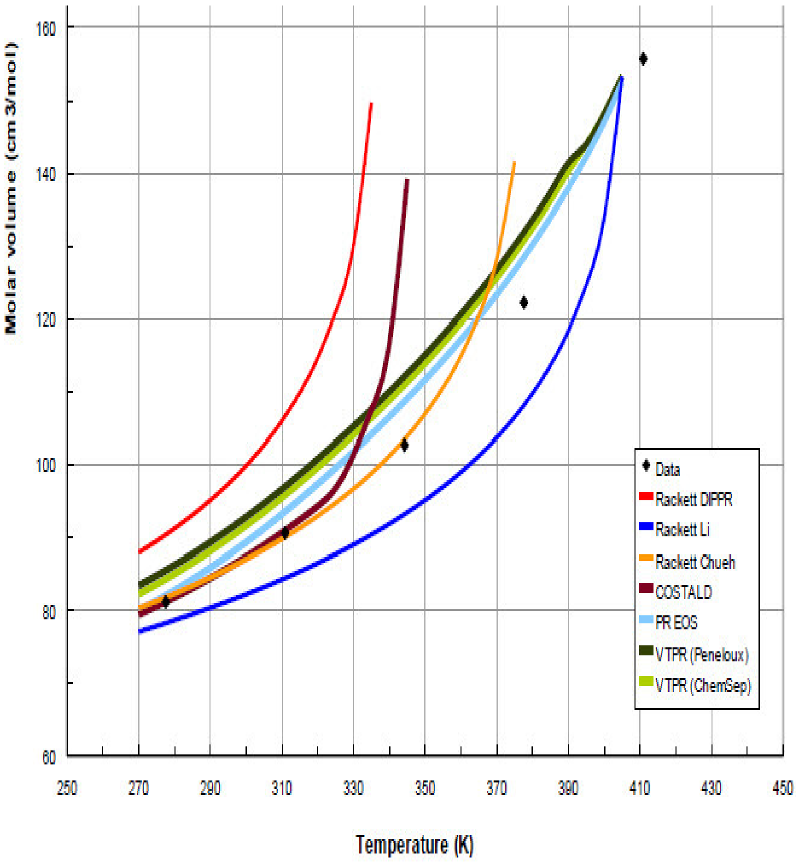


Method	Flooding (tray #)	Weeping (tray #)
Hankinson	4	12 to 14
PR	-	12 & 13
Rackett	3 to 10	12 & 13
Yen-Woods	3 to 9	12 & 13

The Effect of Properties Estimation: Liquid Density Estimation
Capacity Loss due to unexpected flooding



Mixture C2 (10%) - C10



Mixture C2 (90%) - C10

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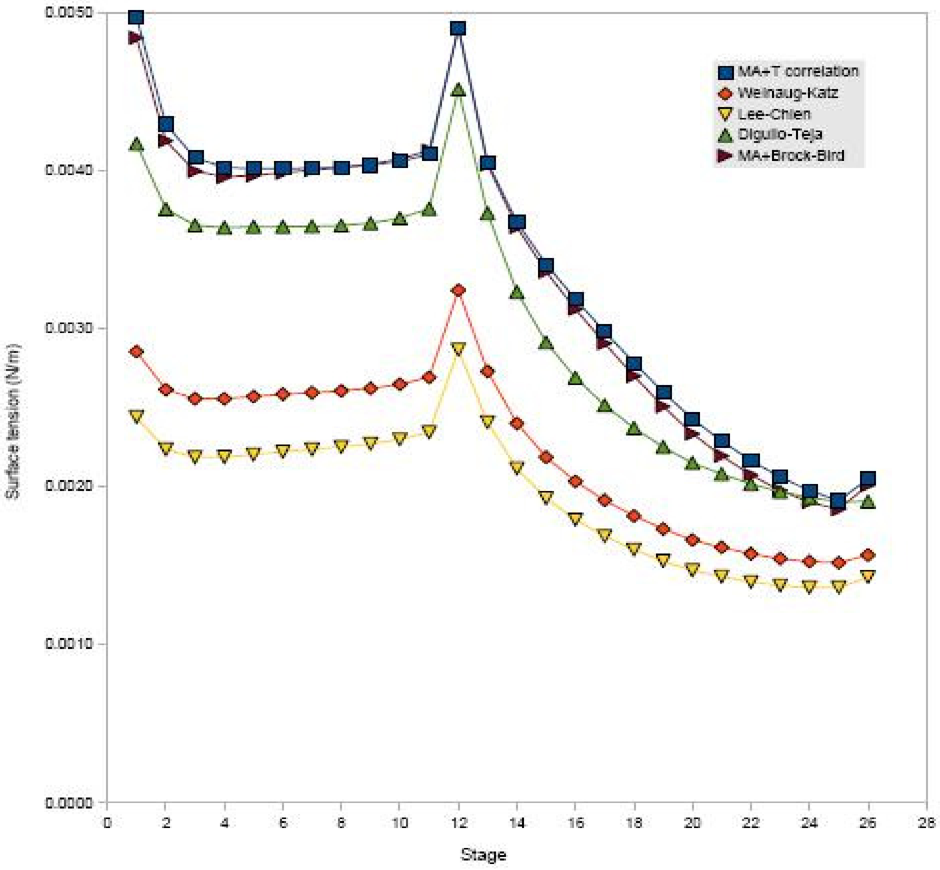
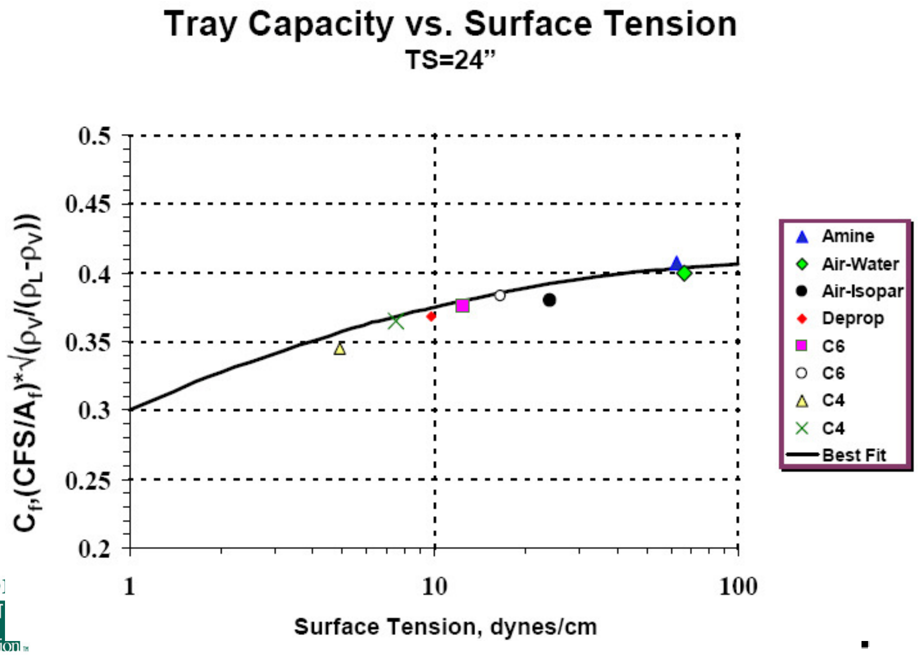
The Effect of Properties Estimation: Surface Tension Estimation
Capacity Loss due to possible flooding



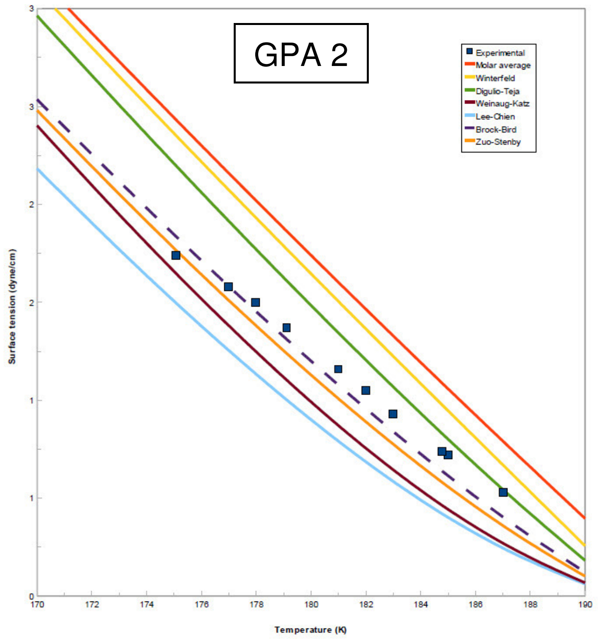
Method	Flooding (tray #)	Weeping (tray #)
MA + T	4	12 to 14
Weinaug-Katz	2 to 10	12 to 14
Lee-Chien	2 to 11	12 to 14
Digulio - Teja	3 to 8	12 to 14
MA+Brock-Bird	3 to 5	12 to 14

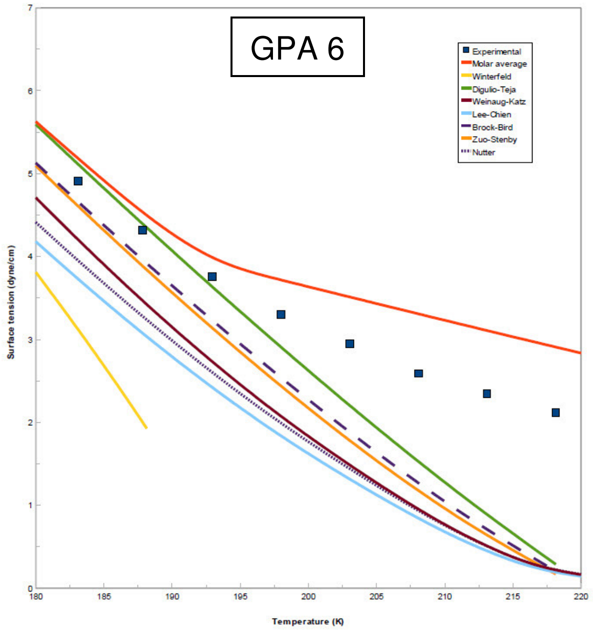

Tray Capacity vs. Surface Tension
TS=24”

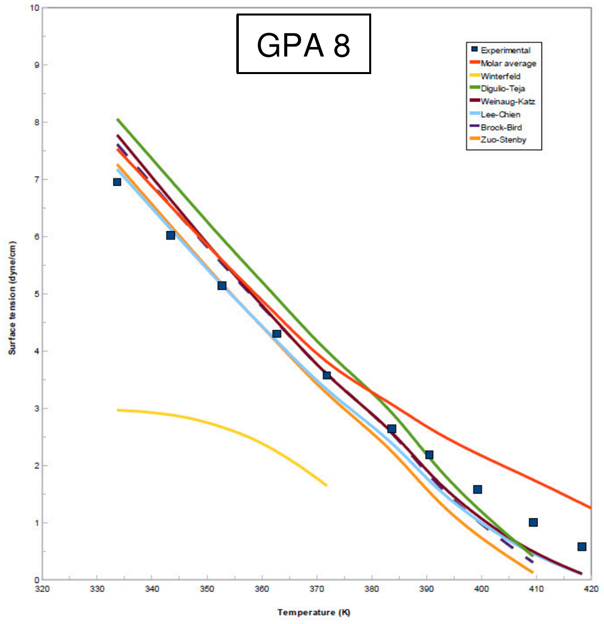
Surface Tension Prediction

Effects on Distillation Towers => Capacity Loss

Compound	GPA 2	GPA 3	GPA 4	GPA 5	GPA 6	GPA 7	GPA 8
Methane	0.989	0.9690	0.9560	0.9110	0.7400	0.01	0
Ethane	0.011	0.0310	0.0440	0.0890	0.2490	0.5	0.03
Propane					0.0110	0.23	0.51
N-butane						0.21	0.32
N-heptane						0.05	0.14







Data from : High Pressure Demethanizer Physical Properties,
S. Horstmann, A. Grybat, C. Ihmels, K. Fischer, GPA Research Report RR-203, 2010

Concluding Remarks and Proposed Next Steps

1. **Rate Base Simulations, based on simultaneous heat and mass transfer, are a tool that can enhance the reliability of new designs and troubleshooting operations.**

2. **Three "Key Ingredients" are the appropriate selection and validation of:**
    - **Equation of State and corresponding BIPs**
    - **Flow Patterns**
    - **Physical Properties Estimation**

3. **Care should still be taken when predicting column performance, even when extrapolating experiences from "similar systems" to "different conditions". Since, "It is not about techniques or technology, it is about how to use them", there is no substitute for caution, knowledge and experience.**

4. ***Efficiency prediction still remains the area where the biggest gains that can be made from further research in distillation.*** *M.J. Lockett, "Distillation Tray Fundamentals"*

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Final Thoughts

Tuning a model requires time and effort.

"Research is the Key to Better Design" ***FRI***