

Application of the New FRI Valve Tray Efficiency Model in Column Simulation and Design

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Ross Taylor - Clarkson University

Attilio J. Praderio - ConocoPhillips - LNG Technology

Special thanks to FRI

Mike Resetarits
Anand Vennavelli

This Presentation:

1. Background – Efficiency concepts through the years
2. Bubble Geometry Efficiency Models (Bubble GEMs)
3. Implementation of FRI model in *ChemSep*
4. Applications of the FRI Model
5. Concluding Remarks

Efficiency Concepts

Equipment design

Mass transfer

Fluid flow model

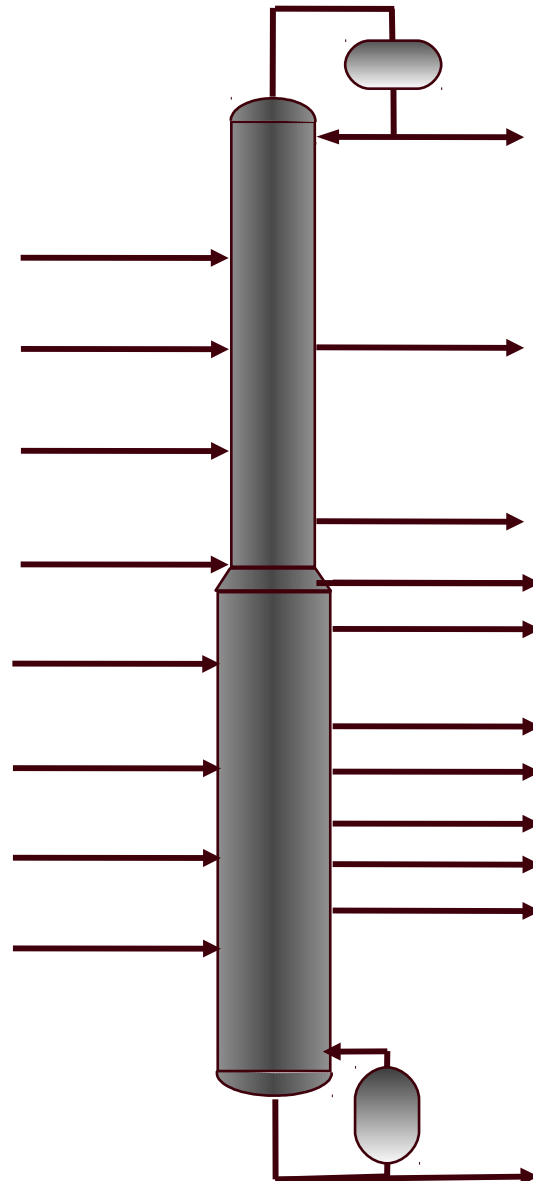
Computational method

Phase equilibrium

Summation equations

Energy balances

Mass balances



Geometric (Baur)

Bubble GEMs

Generalized Hausen (Standart)

AIChE method

Hausen

O'Connell

Vaporization (McAdams) ?

Lewis Cases

Murphree

Overall Efficiency (Lewis)

“Rigorous” Model
(Equilibrium stage)

2000

1900

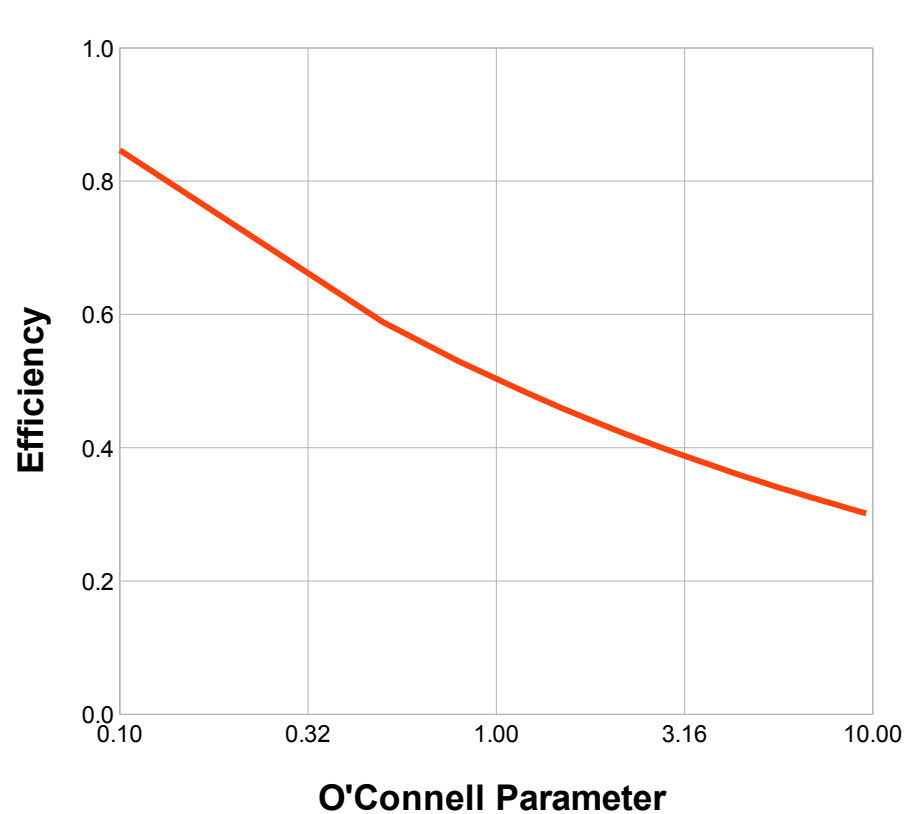


The concept of the theoretical plate does not offer a satisfactory basis for calculation of rectifying columns when the mixture ... contains more than two components.

E.V. Murphree (1925)

$$E_{MV} = \frac{\text{Actual composition change}}{\text{Equilibrium composition change}} = \frac{\Delta y_{i,L}}{\Delta y_i^*}$$

O'Connell Correlation



1942

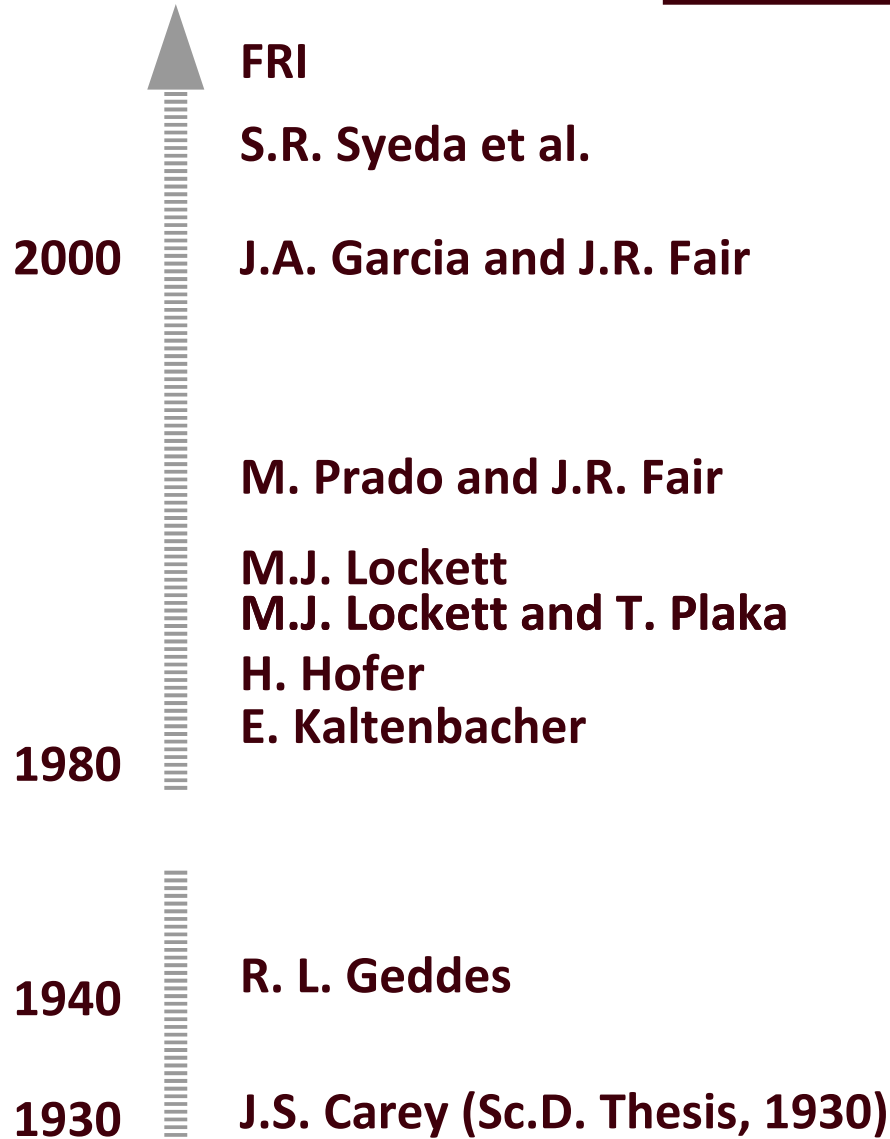
2000

1900

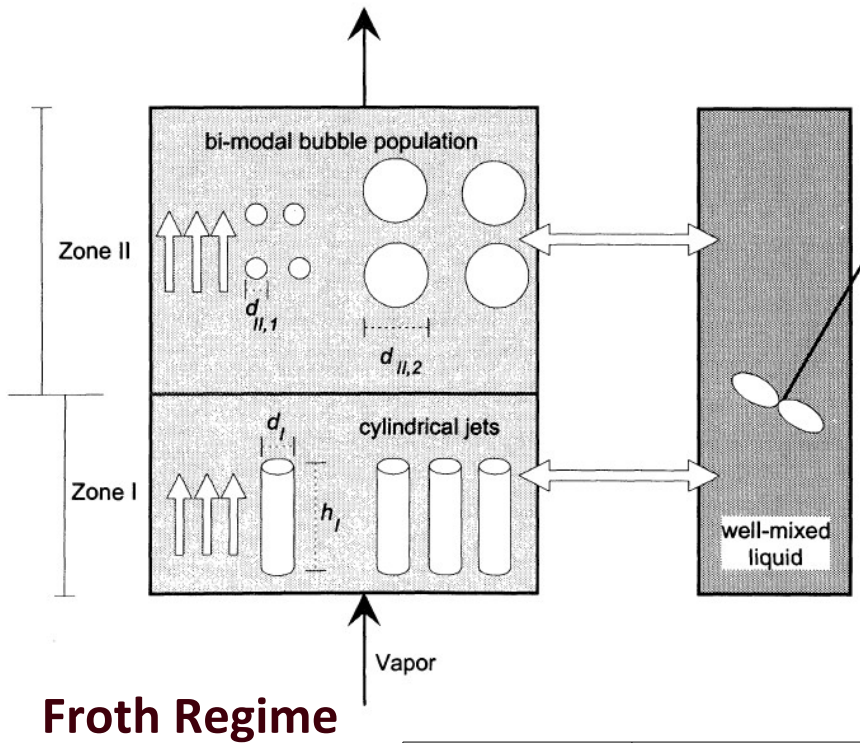
$$E_o = 50.3 (\alpha \mu)^{-0.226}$$

α relative volatility between keys
 μ liquid viscosity in cP

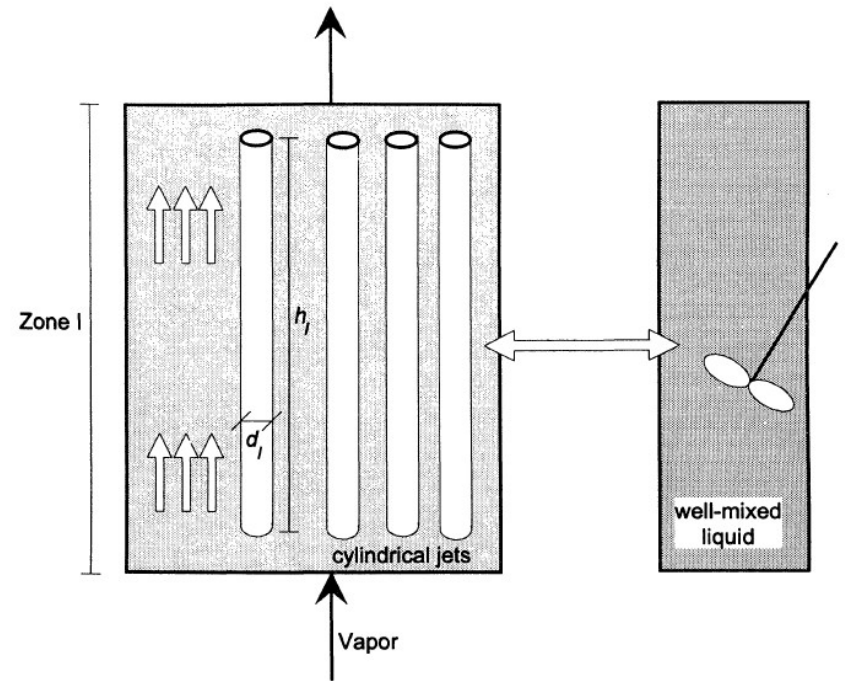
Bubble Geometry Efficiency Models: Milestones



Bubble Geometry Efficiency Models: Physics



Froth Regime

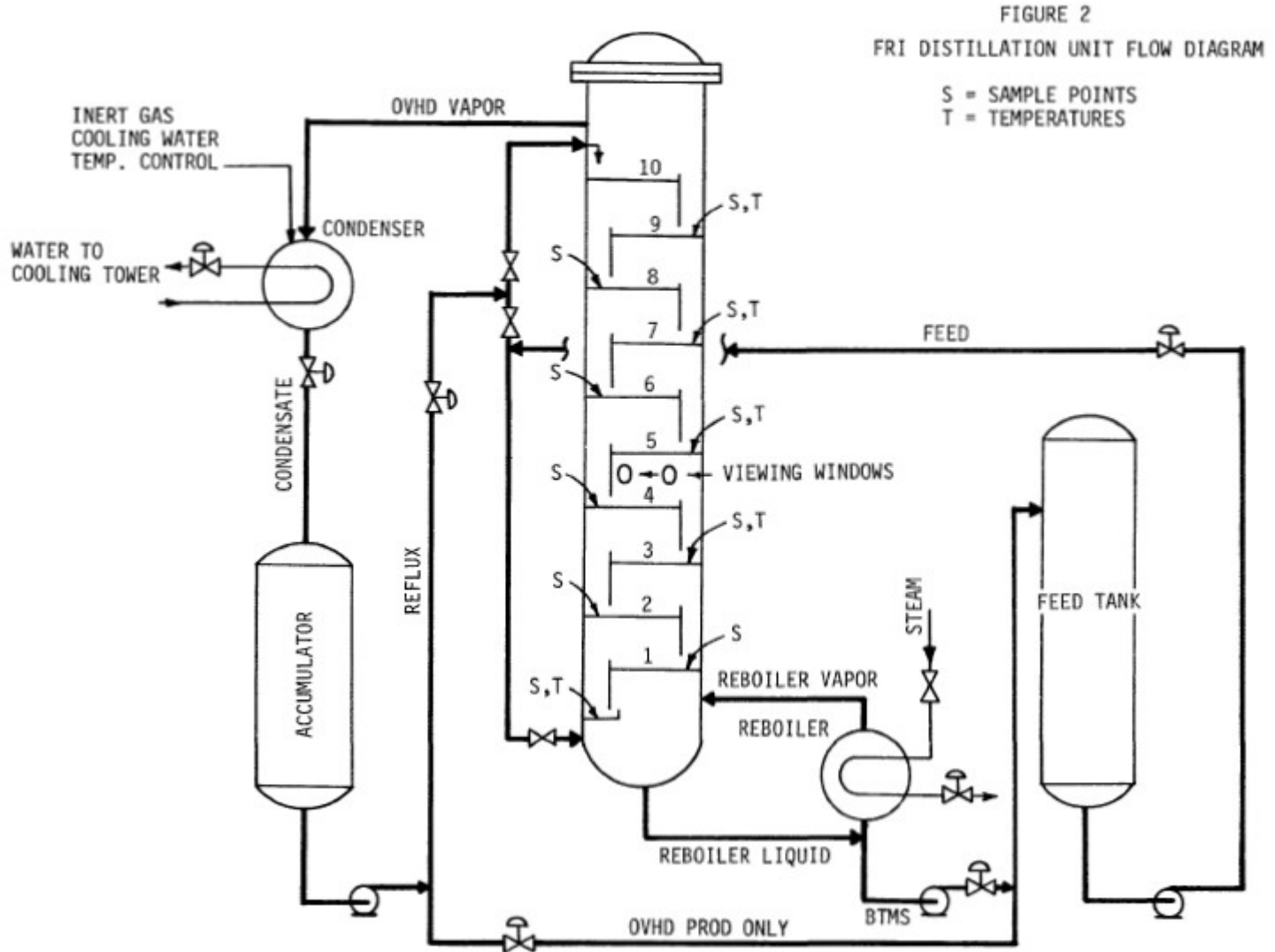


Spray Regime

Zone I	Zone II
Height	Small bubble diameter
Diameter	Large bubble diameter
	Small bubble rise velocity
	Large bubble rise velocity
	Fraction small bubbles

1. FRI Test System I: nC4 – iC4 – C3 @ 165 psia
2. FRI Test System II: o-Xylene – p-Xylene @ 20 mm Hg
3. Industrial Case Study I: C4 splitter
4. Industrial Case Study II: Dehexanizer
5. Design Case Study: BTX column

The FRI Column



Modeling the FRI Column in ChemSep

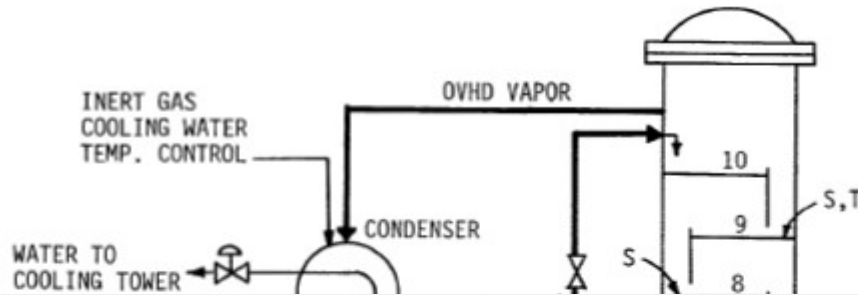


FIGURE 2
FRI DISTILLATION UNIT FLOW DIAGRAM

S = SAMPLE POINTS
T = TEMPERATURES

✓ Operation

Select Type of Simulation

- Flash
- Equilibrium column
- Nonequilibrium column
- Dynamic column

Configuration

Operation: Total Reflux Column

Condenser: Total (Subcooled product)

Reboiler: Total (Vapour product)

Number of stages (e.g. 10): 12

Feed stage(s) (e.g. 5,7): 7

Sidestream stage(s) (e.g. 2,9):

Pumparound(s) (e.g. 6>8, 9>1):

FEED

Total Reflux Compositions

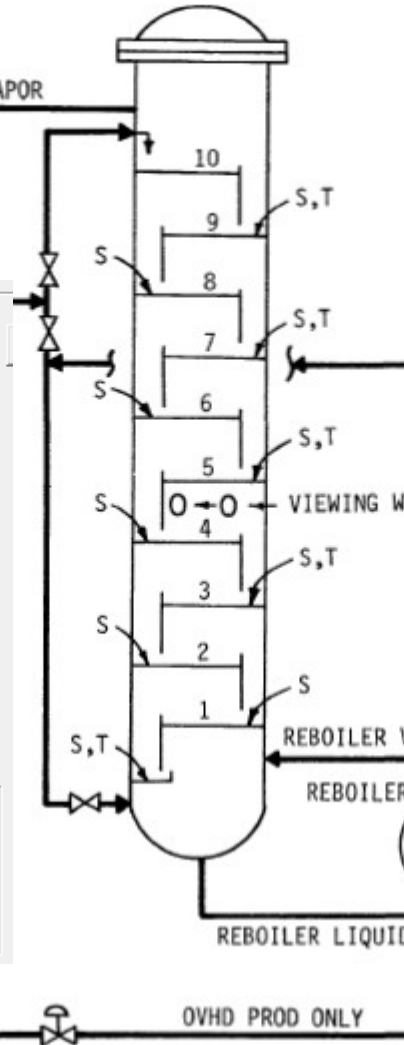
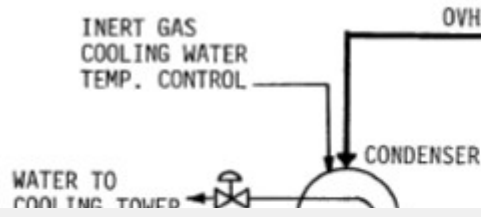
Stage	7
State	Liquid
Mole fractions:	
N-butane	0.585500
Isobutane	0.414200
Propane	3.0000E-04
Total	1.00000
Internal flow	Reflux (mass)
Flowrate (lb/h):	15.7000
Condenser	Qcondenser
Reboiler	Qreboiler
Subcooling (K)	Temperature of reflux
Superheating (F)	324.817

BOILER VAPOR

LIQUID

BTMS

Modeling the FRI Column in ChemSep



Internals Design

Insert Remove Copy System factor 1.00000

Section	1 (rating)
Column internals	Valve tray
First stage	2
Last stage	11
Section height (m)	6.09600
Mass transfer coefficient	Equilibrium Stage
Liquid phase resistance	Included
Vapour flow model	Mixed flow
Liquid flow model	Mixed flow
Pressure drop	Fixed
Entrainment	None
Holdup	
Design method	Fraction of flood

Section 1 Column internals: Valve tray

Load Save Reset

Column diameter (m)	1.21920
Tray spacing (mm)	609.600
Number of flow passes	1.00000
Liquid flow path length (mm)	787.400
Active area (m2)	0.888153
Total hole area (m2)	0.135220
Downcomer area (m2)	*
Hole diameter (mm)	12.7000
Hole pitch (mm)	*
Weir length (m)	0.939800
Weir height (mm)	63.5000
Weir type	Segmental
Notch depth/Weir diameter (mm)	*
Serration angle (rad)	*
Downcomer clearance (mm)	*
Deck thickness (mm)	1.98000
Downcomer sloping	*
Downcomer length	*
Closed Loss K	*
Open Loss K	*
Eddy Loss C	*
Ratio Valve Legs	*
Valve Density	7680.00
Valve Thickness	*
Fraction Heavy Valves	0.000000
Heavy Valve Thickness	*

Internals Design

Insert Remove Copy System factor 1.00000

Section	1 (rating)
Column internals	Valve tray
First stage	2
Last stage	11
Mass transfer coefficient	Equilibrium Stage
Vapour flow model	Mixed flow
Liquid flow model	Mixed flow
Pressure drop	Fixed
Entrainment	None
Holdup	
Design method	Fraction of flood

Section 1 Mass transfer coefficient: Modified O'Connell

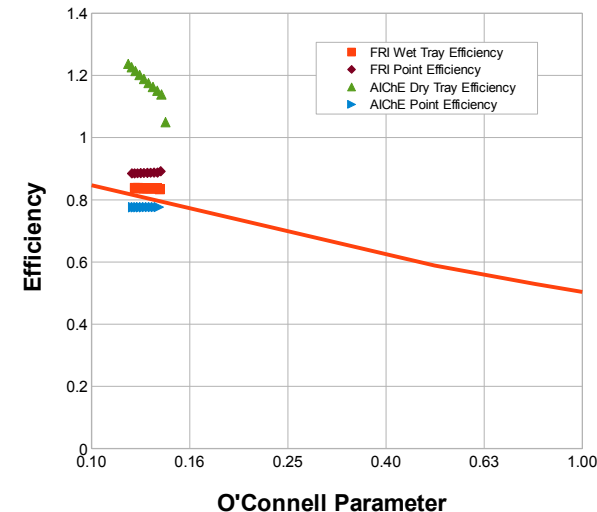
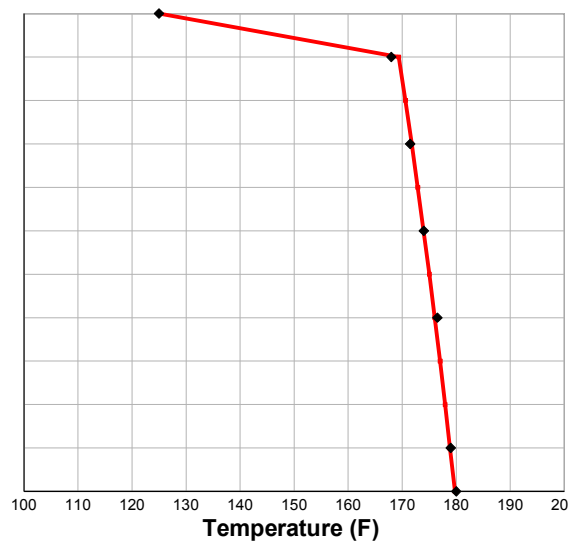
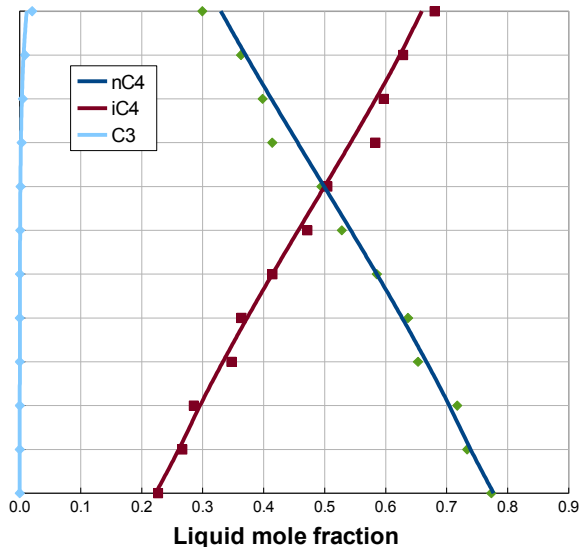
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Efficiency	Modified O'Connell
Light Key	Isobutane
Heavy Key	N-butane
Modified O'Connell Slope	*
Modified O'Connell Intercept	*

FRI Test 9276: n-C4 – iC4 – C3 @ 165 psia

<p>Tray Type</p> <p>Valves</p> <p>Tray spacing</p> <p>Weir length</p> <p>Weir height</p> <p>Downcomer Area</p>	<p>Glitsch Ballast Tray</p> <p>114 V-0 units</p> <p>24 in</p> <p>37 in</p> <p>2.5 in</p> <p>1.5 ft²</p>
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	TR 041	Simulation
Condenser Duty (MM Btu/h)	2.56	2.33
Reboiler Duty (MM Btu/h)	2.30	2.33
Tray 4 liquid density (lb/ft ³)	30.7	30.5
Tray 4 vapor density (lb/ft ³)	1.78	1.81
Tray Efficiency (%)	91.9	83.7

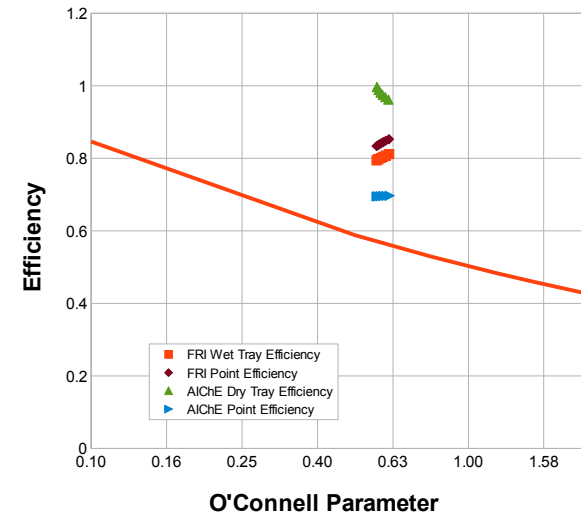
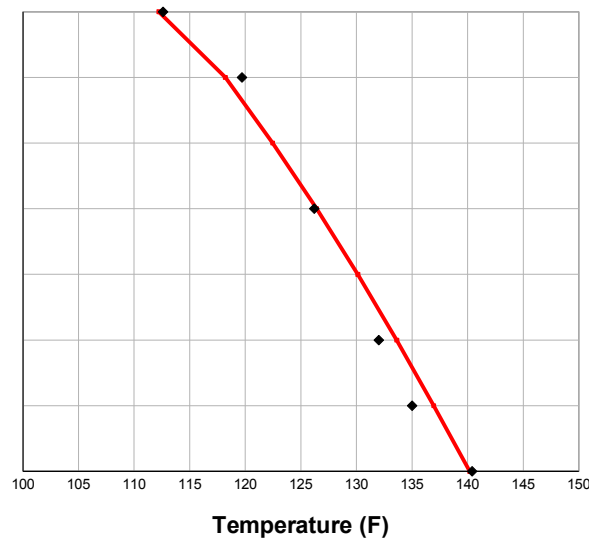
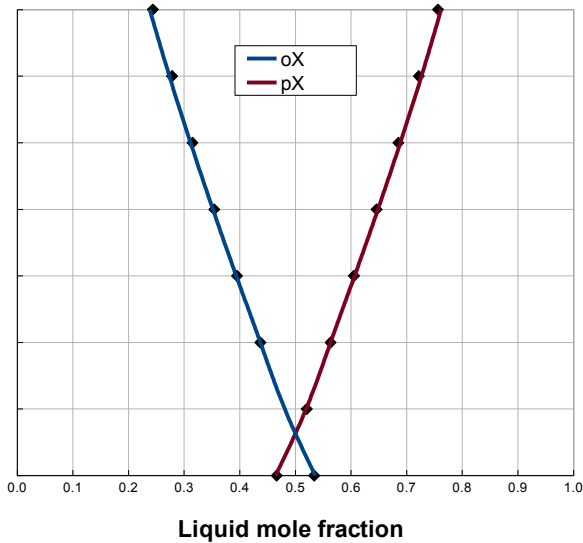


Composition and temperature profiles with FRI tray efficiency model.

FRI Test 9346: o-Xylene – p-Xylene @ 20 mmHg

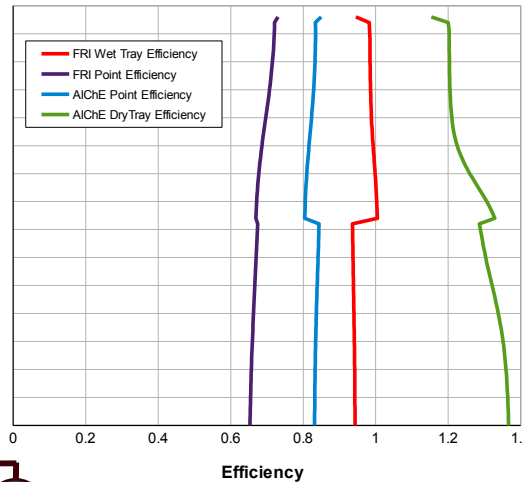
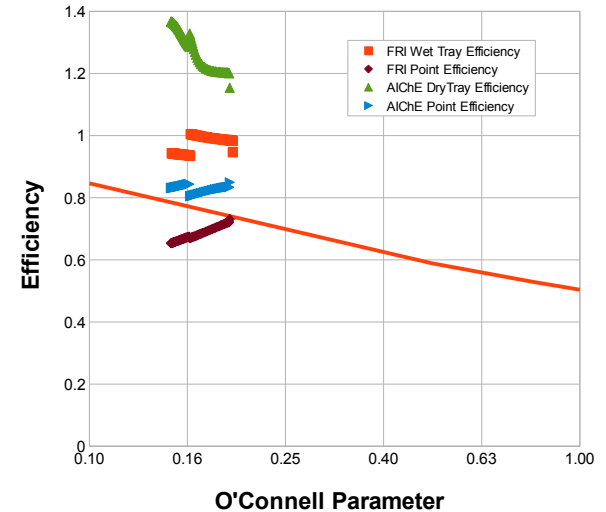
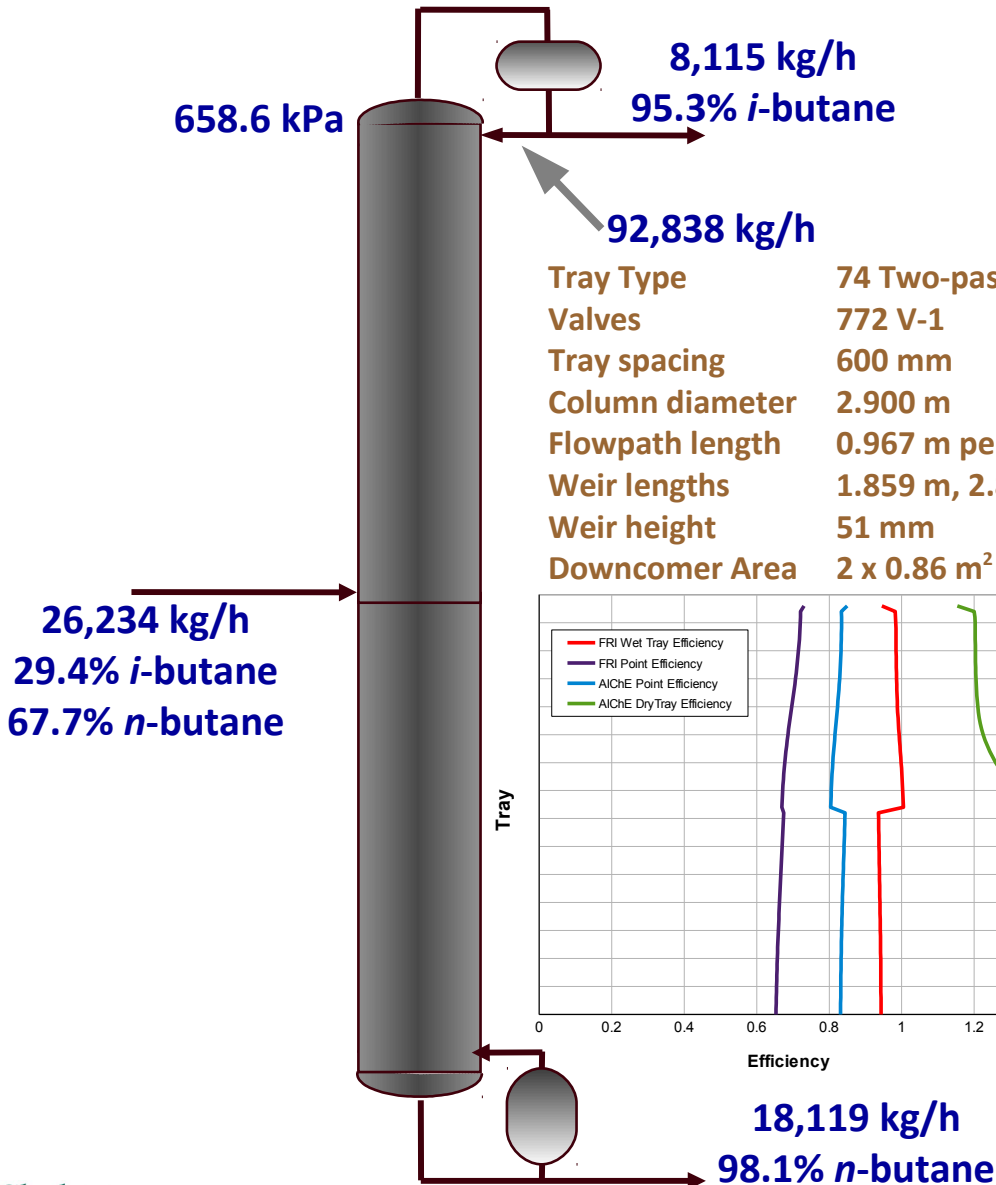
<p>Tray Type</p> <p>Valves</p> <p>Tray spacing</p> <p>Weir length</p> <p>Weir height</p> <p>Downcomer Area</p>	<p>Koch Flexitray Type T</p> <p>167 double weight</p> <p>24 in</p> <p>30 in</p> <p>0.75 in</p> <p>0.53 ft²</p>
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	TR 044	Simulation
Condenser Duty (MM Btu/h)	0.976	0.941
Reboiler Duty (MM Btu/h)	0.934	0.941
Tray 2 liquid density (lb/ft ³)	52.4	52.3
Tray 2 vapor density (lb/ft ³)	0.0122	0.0139
Tray Efficiency (%)	77.0	79.4-81.5



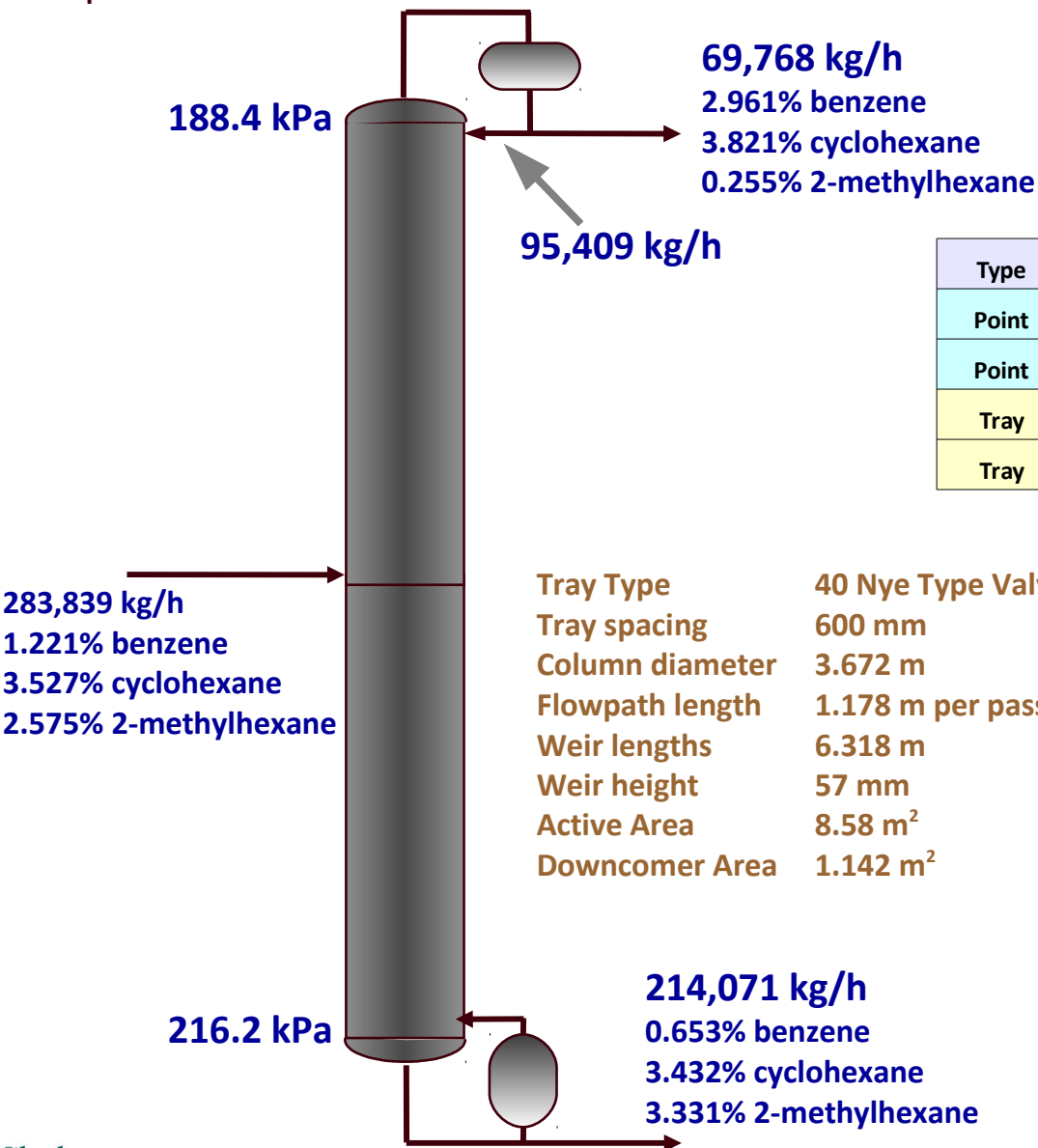
Composition and temperature profiles with FRI tray efficiency model.

C4 Splitter

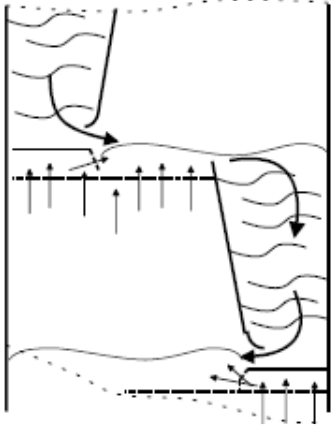


Type	Value(%)	NTU Model	Thermo	Source
Overall	111		SRK	Ilme Ph.D. thesis
Overall	119		UNIFAC	Klemola + Ilme
Overall	114		PR	Taylor and Kooijman
Point	75-82	AIChE	UNIFAC	Klemola + Ilme
Point	81-85	AIChE	SRK	This work
Point	66-75	FRI	SRK	This work
Tray	115-120	AIChE	UNIFAC	Klemola + Ilme
Dry Tray	115-137	AIChE	SRK	This work
Wet Tray	93-101	FRI	SRK	This work

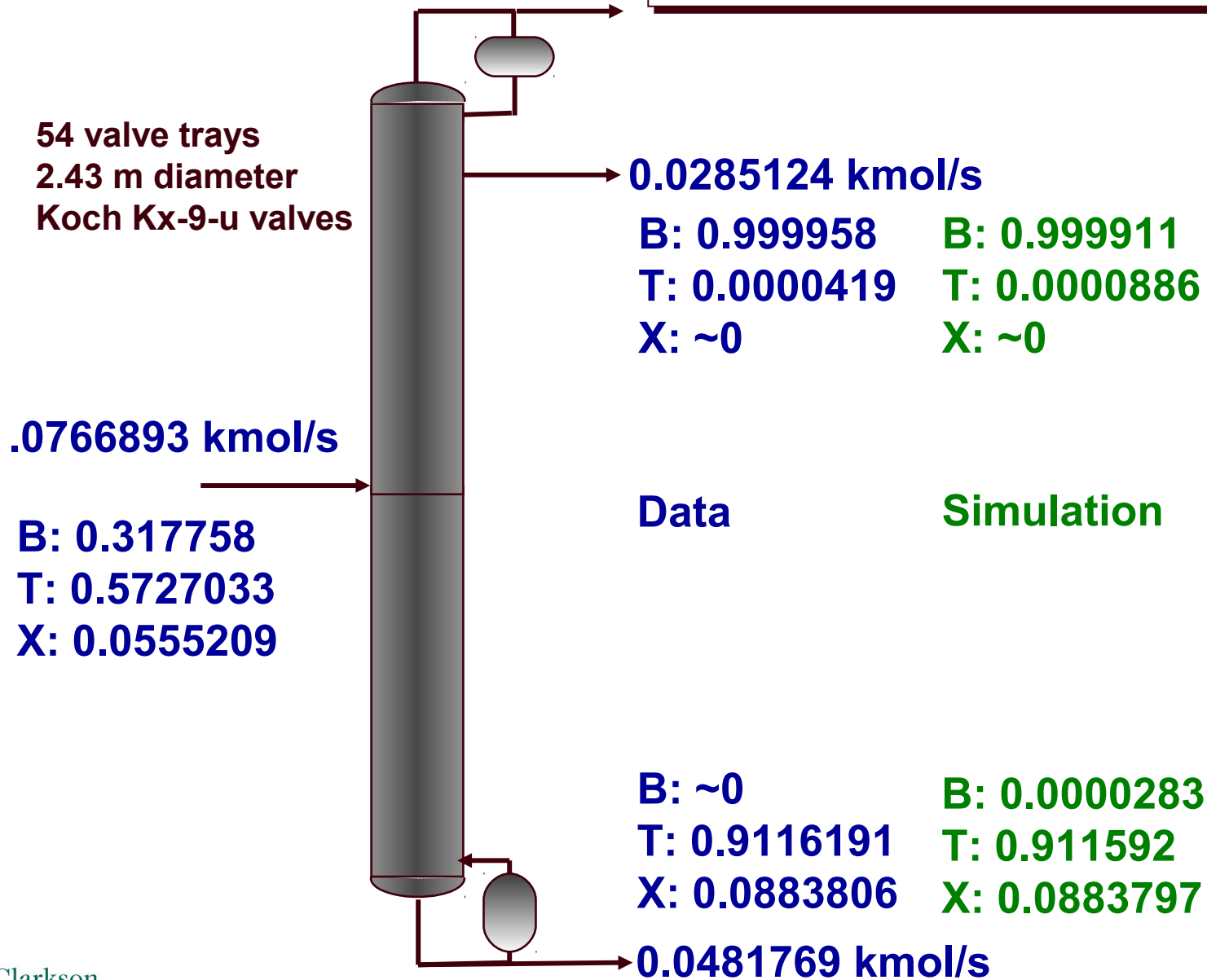
Dehexaniser



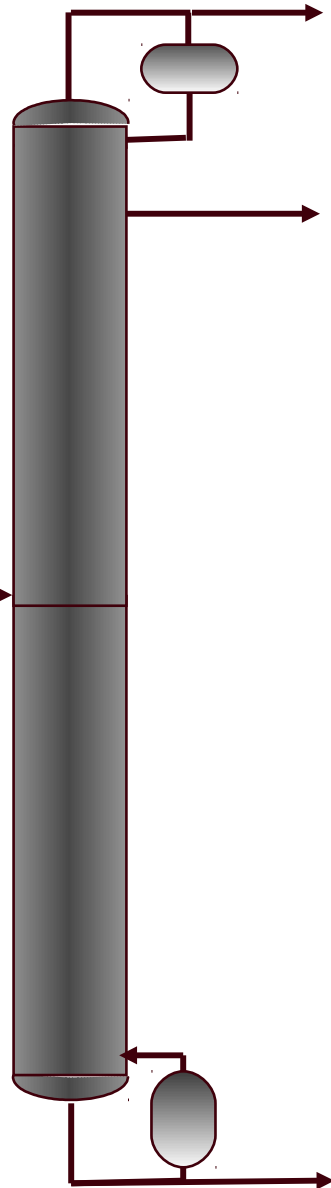
Type	Value(%)	NTU Model	Thermo	Source
Point	75-85	Chan + Fair	SRK	Jakobsson et al.
Point	75-97	AICHe	SRK	This work
Tray	85-110	Chan + Fair	SRK	Jakobsson et al.
Tray	80-110	FRI	SRK	This work



Design Case Study: BTX Column



Design Case Study: BTX Column



54 valve trays
2.43 m diameter
Koch Kx-9-u valves

.0766893 kmol/s

B: 0.317758
T: 0.5727033
X: 0.0555209

Select table: Internals design

XLS

Edit

Copy

Font

Tray design produced by ChemSep.

Column design:

FRI model used only for efficiency, not for tray sizing.

Number of sections	1
Default system factor ()	0.900000
Section	1
Column internals	Valve
First stage	2
Last stage	55
Flood limit @stage	65% jf @26
Section height (m)	
Column diameter (m)	2
Tray spacing (mm)	610
Number of flow passes	2
Liquid flow path length (mm)	748.429
Active area (m ²)	2.57507
Total hole area (m ²)	0.630425
Downcomer area (m ²)	0.283258
Hole diameter (mm)	50.8
Hole pitch (mm)	97.8704
Weir length (m)	2.30029
Weir height (mm)	54.08
Weir type	Segmental
Notch depth/Weir diameter (mm)	*
Serration angle (rad)	*
Downcomer clearance (mm)	41.38
Deck thickness (mm)	2.54
Downcomer sloping	0
Downcomer length	1
Closed Loss K	0.8413
Open Loss K	0.1225
Eddy Loss C	1.3
Ratio Valve Legs	1.29
Valve Density	7849
Valve Thickness	0.003
Fraction Heavy Valves	0
Heavy Valve Thickness	0

jf=jet flood, dv=downcomer velocity, bu=Backup, ck=Downcomer choking
sl=system limit, wl=weir loading, rt=residence time
wp=weeping/insufficient wetting, dp=dumping/unsealing, sb=stability

Concluding Remarks and Proposed Next Steps

1. Bubble GEMs are comprehensive models of tray efficiency that separate the contributions to mass transfer from jetting and different bubble populations. This separation permits the systematic exploration of mass transfer in different flow regimes.
2. FRI valve tray efficiency model is *complete* (in that the model is self-contained).
3. FRI model was implemented as an “added model” for *ChemSep*.
4. Tests of the *ChemSep* implementation show very good match with FRI distillation data at total reflux.
5. Tentative: Simulations of some commercial scale processes suggest that the FRI model is not able to match the observed overall efficiencies so well.
6. FRI model can be used at the design stage.
7. FRI model should be extended to sieve trays.
8. Column profile data for operations *not* at total reflux would be useful.

Bubble Geometry Efficiency Models: References

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Vennavelli, A.N., Whitely, J.R. & Resetarits, M.R. New Fraction Jetting Model for Distillation Sieve Tray Efficiency Prediction, *Ind. Eng. Chem. Res.*, 51, 11458-11462 (2012)