

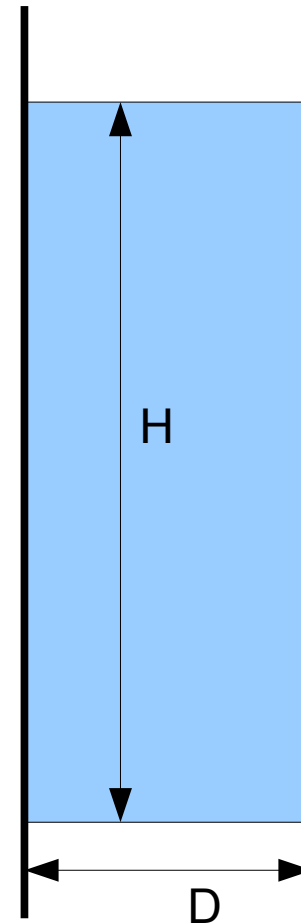
Benchmarking Mass Transfer Correlations with a Nonequilibrium Model

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Packed Column Design

- Column Diameter:
 - Capacity: F-factor or C-factor
 - Pressure Drop: $HETP/\Delta p$
- Column Height
 - Mass Transfer: HETP

*Which models to use for
a particular packing?*



Recent new MTC Models

- Olujic-Delft 1997-2003 [Various]
- Erasmus-Nieuwoudt [IECR, 40, pp.2310-2321]
- Del Carlo-Olujic-Paglianti 2006 [IECR, 45, pp.7967-7976]

How good are these models?

Traditional MTC Model Development

- Total Reflux data (FRI, SRP, TU Delft, Koch-Glitsch, Sulzer ChemTech, ...)
- Simulation with equilibrium model:
 - Determine number of stages
 - Plot average HETP versus F or C-factor
 - Plot pressure drop versus F or C-factor
- Correlate HETP using:
 - One or two-film approach
 - Fixed physical properties

Distillation Test Data

- Typical Systems, Pressures, Thermodynamics:
 - ***c-C6/n-C7, 0.3-4.1 bar, UNIFAC+Antoine***
 - o/p-Xylene, 0.1-0.3 bar, Ideal+Antoine
 - iC4/nC4, 7-11 bar, SRK or PR
 - EB/CB, 0.1 bar, Ideal+Antoine
 - EB/ST, 0.1 bar, Ideal+Antoine
 - MeOH/H₂O, 1 bar, NRTL+Antoine

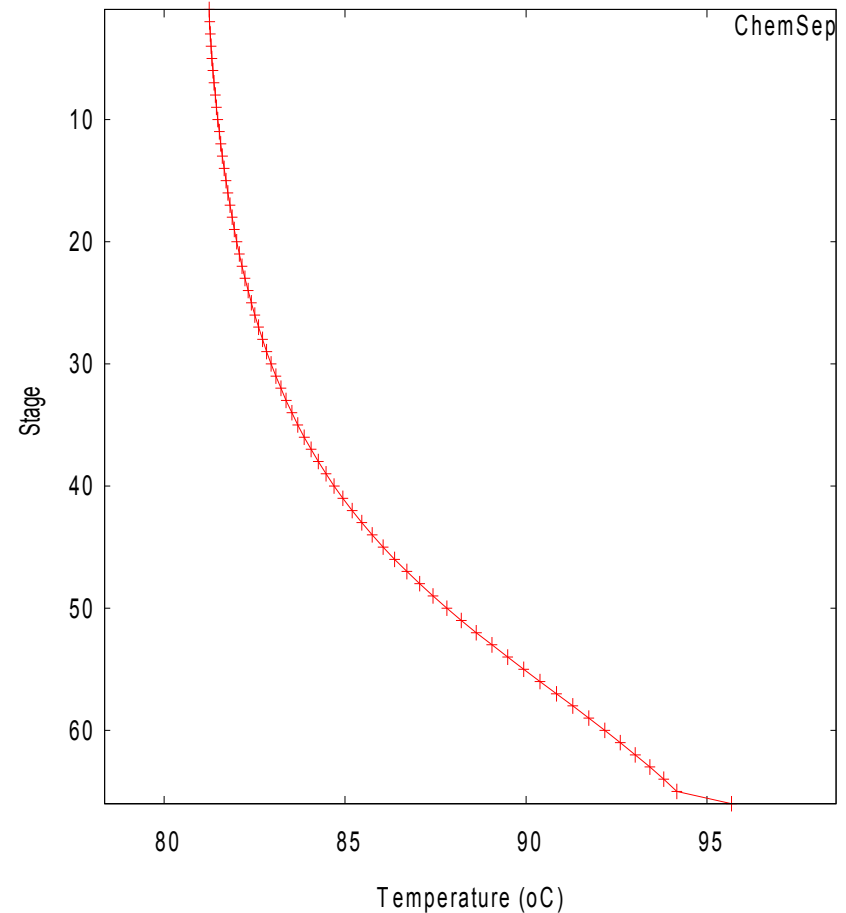
How constant is the HETP?

HETP vs. Packed Bed Height

HETP varies due to:

- T & p changes

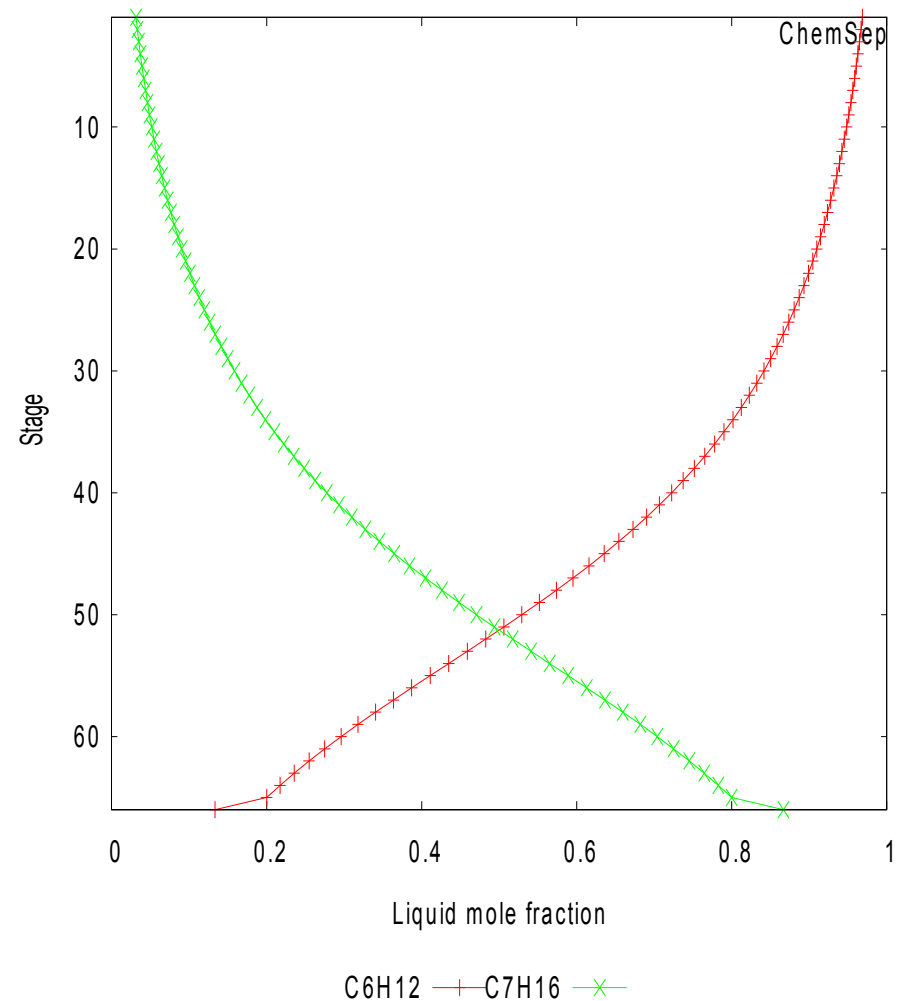
c-C6/n-C7 1atm, 3m bed



HETP vs. Packed Bed Height

HETP varies due to:

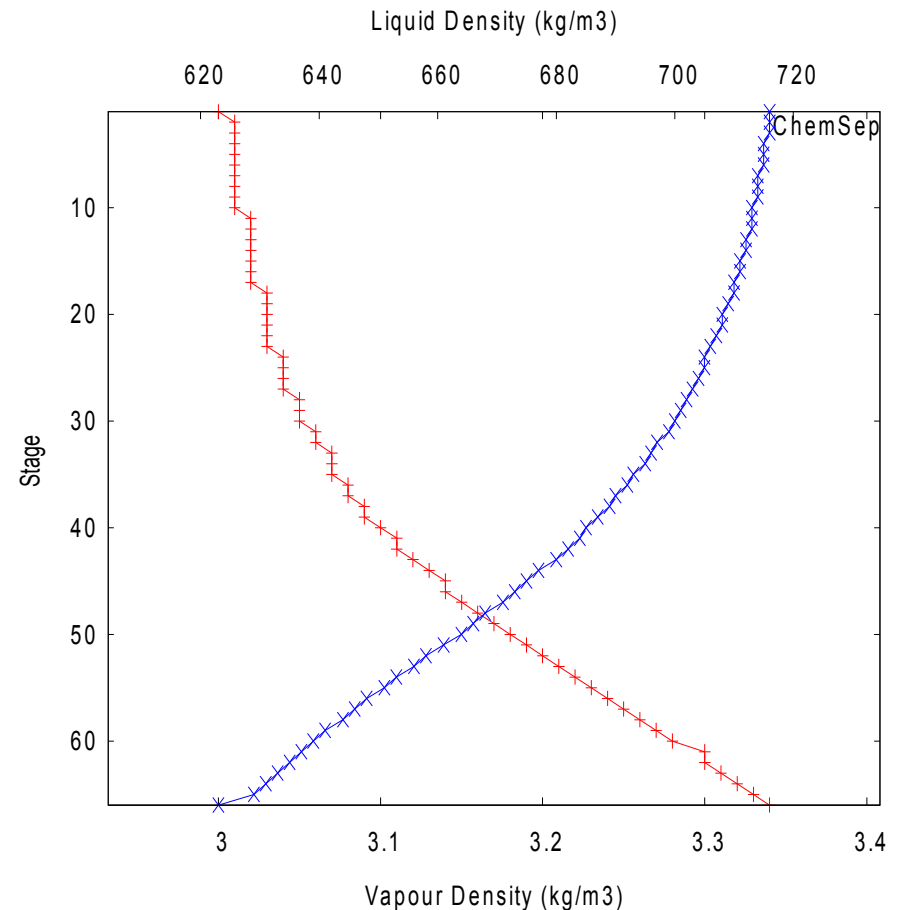
- T & p changes
- Concentration changes



HETP vs. Packed Bed Height

HETP varies due to:

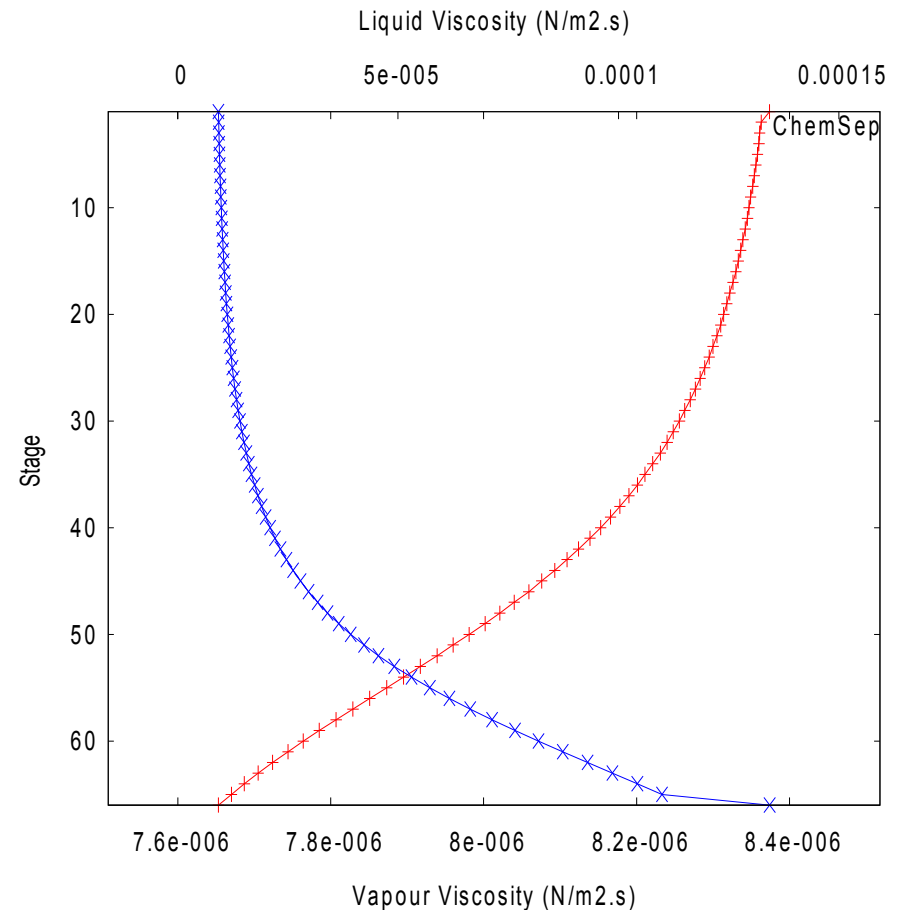
- T & p changes
- Concentration changes
- Consequent changes in densities



HETP vs. Packed Bed Height

HETP varies due to:

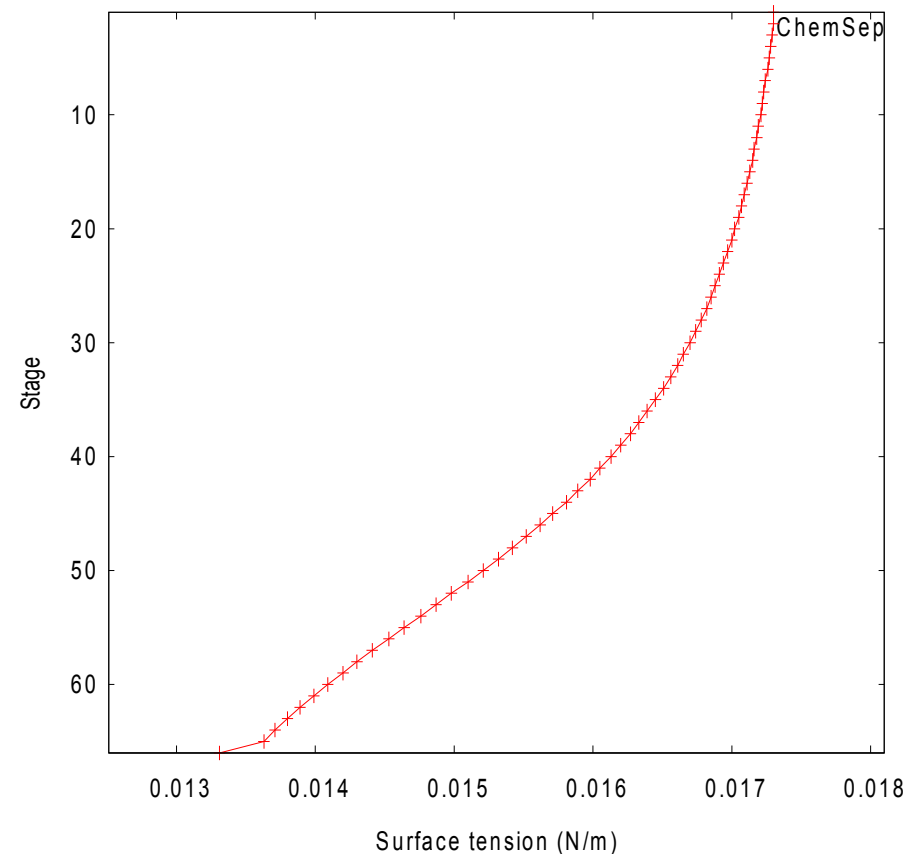
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities



HETP vs. Packed Bed Height

HETP varies due to:

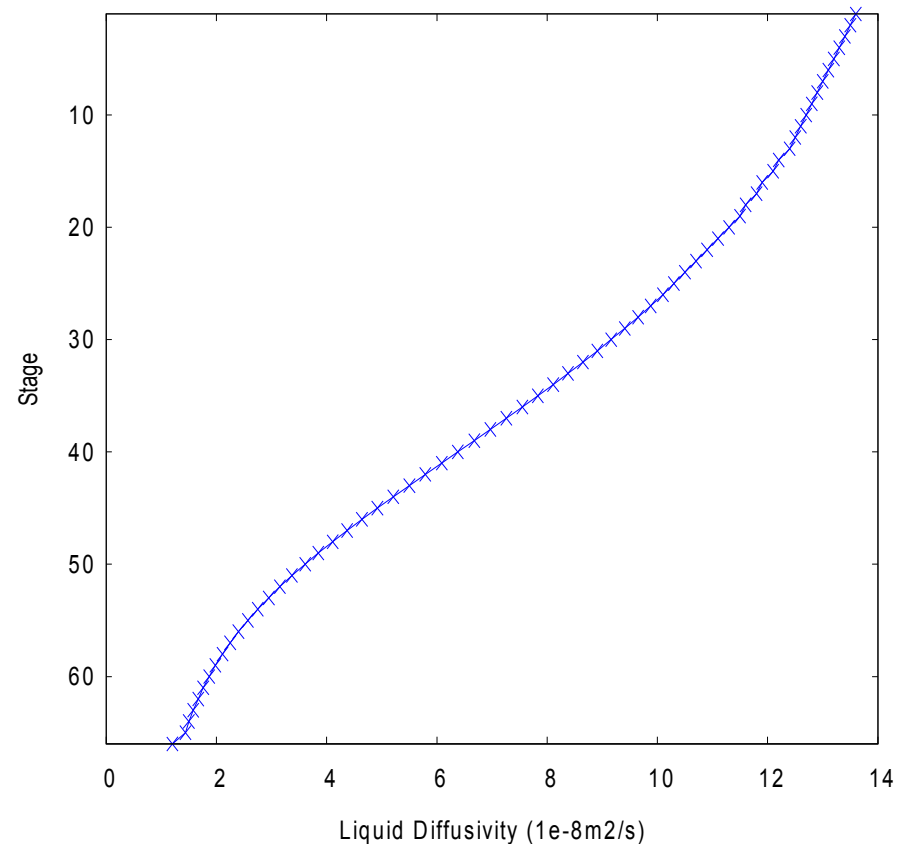
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension



HETP vs. Packed Bed Height

HETP varies due to:

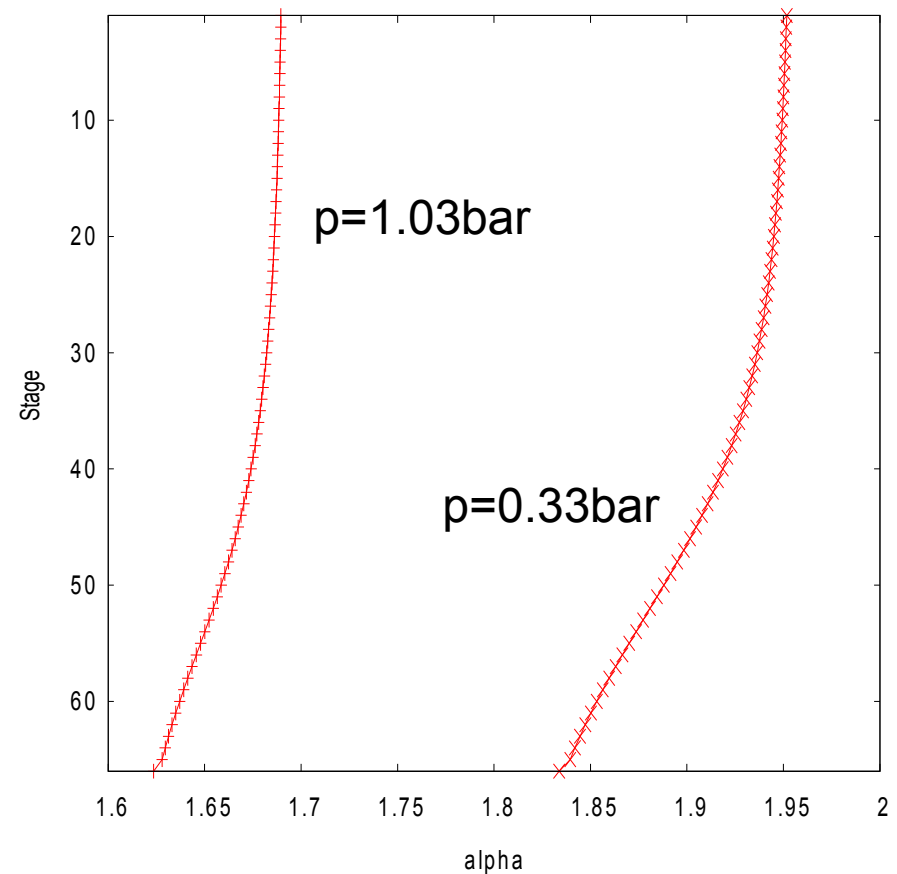
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities



HETP vs. Packed Bed Height

HETP varies due to:

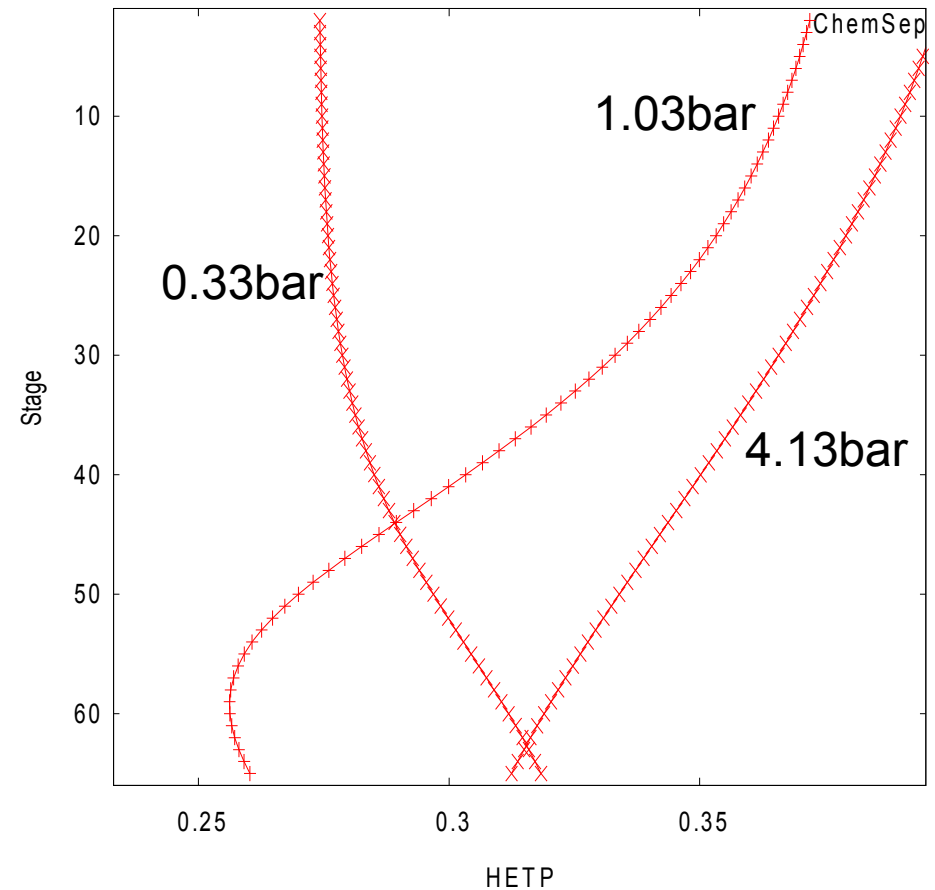
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities
- And changes in relative volatility



HETP vs. Packed Bed Height

HETP varies due to:

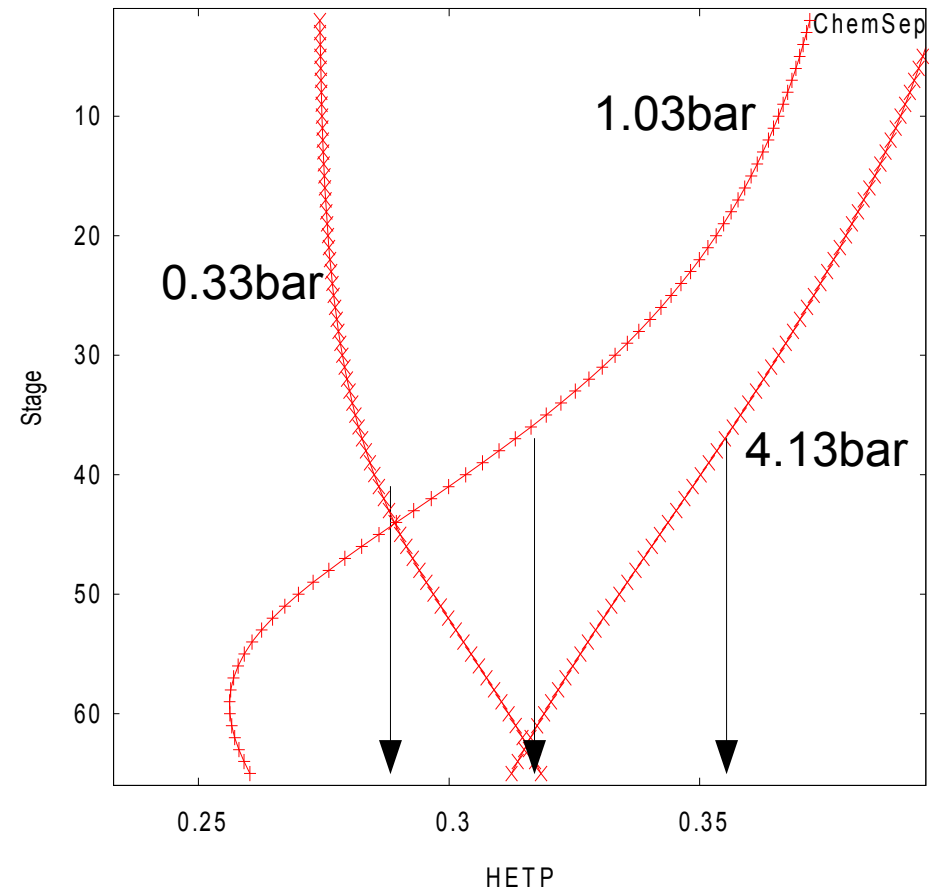
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities
- And changes in relative volatility



HETP vs. Packed Bed Height

HETP varies due to:

- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities
- And changes in relative volatility



**We must average HETP
over the bed height!**

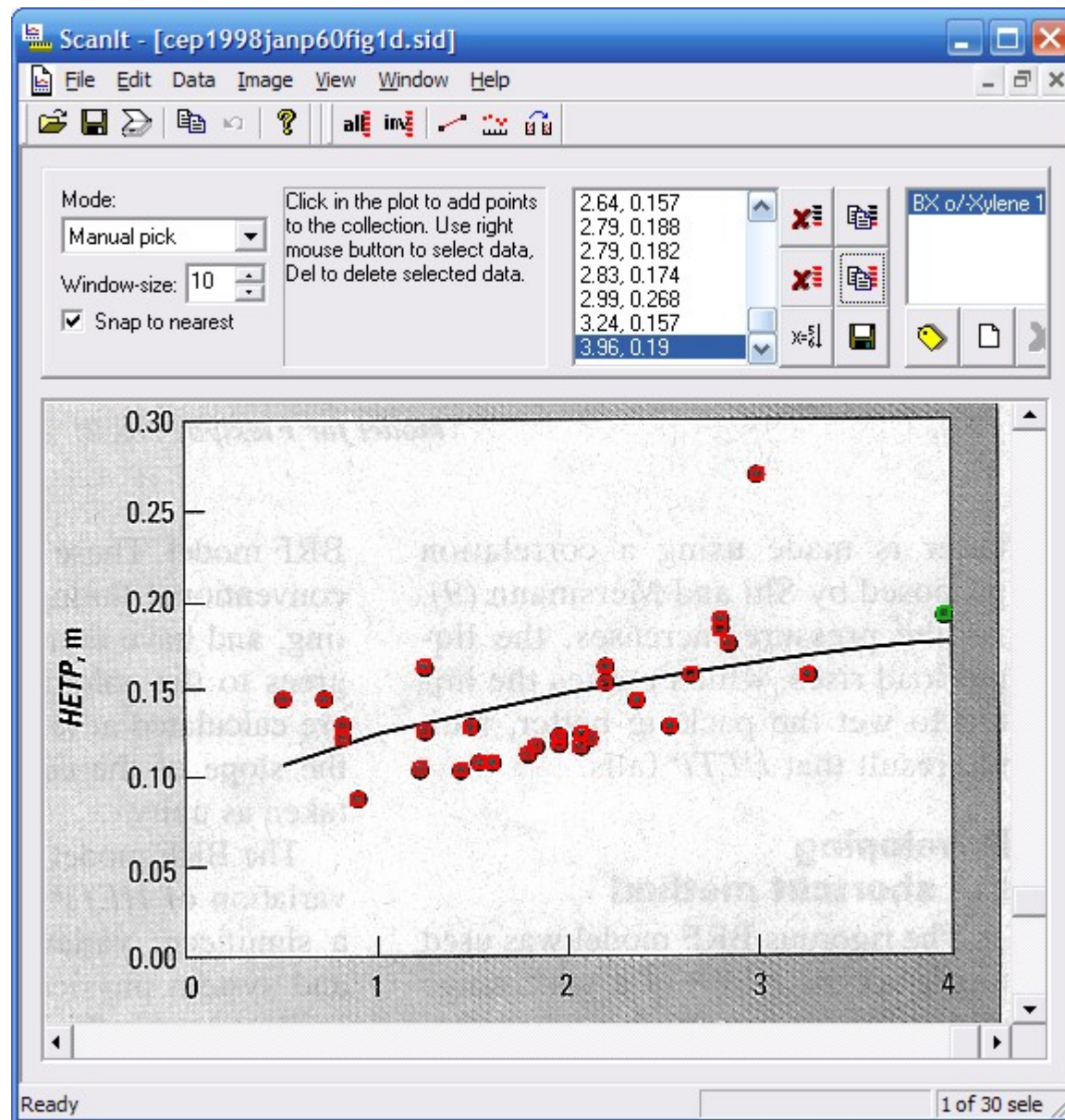
A Different Approach

- Data for multiple systems/pressures
- Simulate in nonequilibrium model (ChemSep)
- Compute HETP from back-calculated efficiency
- Average HETP over the whole packed bed

Problem: Often no concentration gradient published. Use educated guess from T & p

Collecting Data

- “ScanIt”



Collecting Data

- “ScanIt”
- Simulate it:
ChemSep
Total Reflux

The screenshot displays the ChemSep software interface for a Total Reflux Column simulation. The window title is "ChemSep - c6c7_4.13bar_B1-250M_BS92_HETPs.sep - Total Reflux Column". The interface includes a menu bar (File, Edit, Run, Analysis, Databanks, Tools, Help) and a toolbar with icons for file operations and simulation. A left-hand tree view shows the simulation setup, with "Design" and "Total Reflux" selected. The main area is titled "Internals Design" and contains a table of column parameters and a "Section 1: Column internals" table.

Section	1 (rating)
Column internals	Structured Packing
First stage	2
Last stage	65
Section height (m)	3.2
Mass transfer coefficient	Billet-Schultes 1992
Liquid phase resistance	Included
Vapour flow model	Plug flow
Liquid flow model	Plug flow
Pressure drop	Stichmair-Bravo-Fair 1989
Entrainment	None
Holdup	Default
Design method	Fraction of flood

Section 1: Column internals	
Column diameter (m)	0.43
Stage height (m)	0.05
StructuredType	Montz B1-250 M
Specific surface area (m ²)	244
Structured void fraction (m ³)	0.98

Collecting Data

- “ScanIt”
- Simulate it:
ChemSep
Total Reflux
- Parametric Study to plot
average HETP
vs F-factor

The screenshot shows the 'Parametric Study' dialog box with the following details:

Select input variables:

- Number of steps: 6
- Use old results:
- Automatic:
- Keep sep-files:
- Restore original:

Name	Variable	Units	Value	Start/Valuelist	End
Reflux liquid flow	RL	mol/s	9	3	9

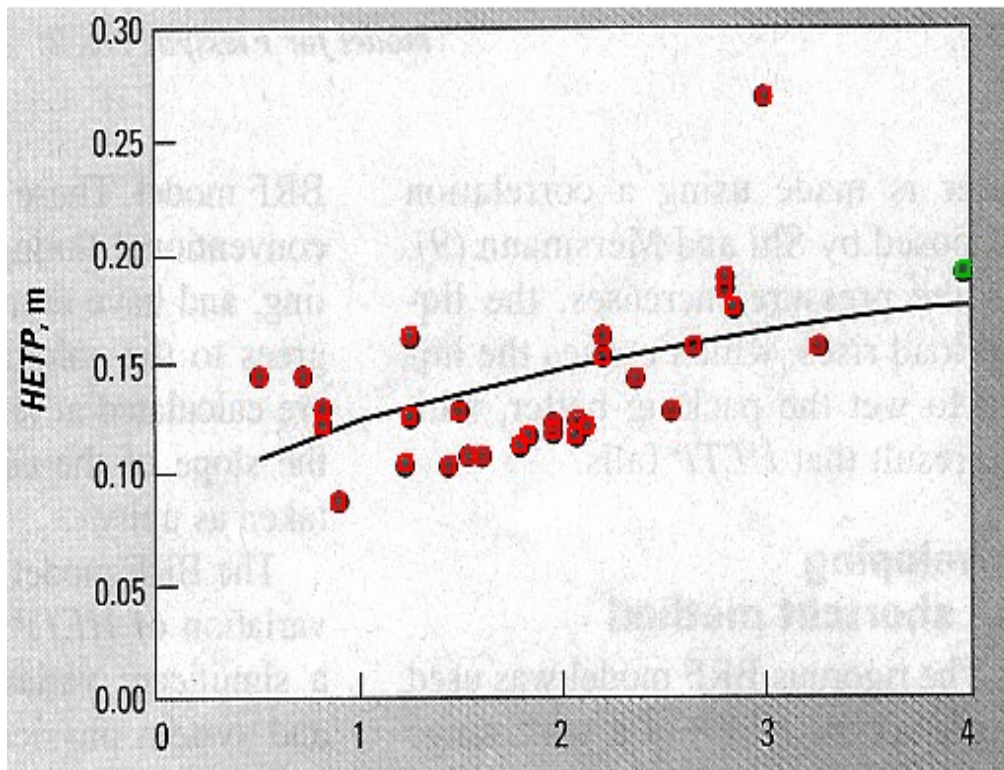
Select result variables:

Name	Reflux liquid flow	F-factor	AHETP1	pd (mbar/m)
Variable	RL	FFAC35	AHETP1	(P65-P1)/300
Units	mol/s			
Current Value	9	3.129096	0.316537	1.260937

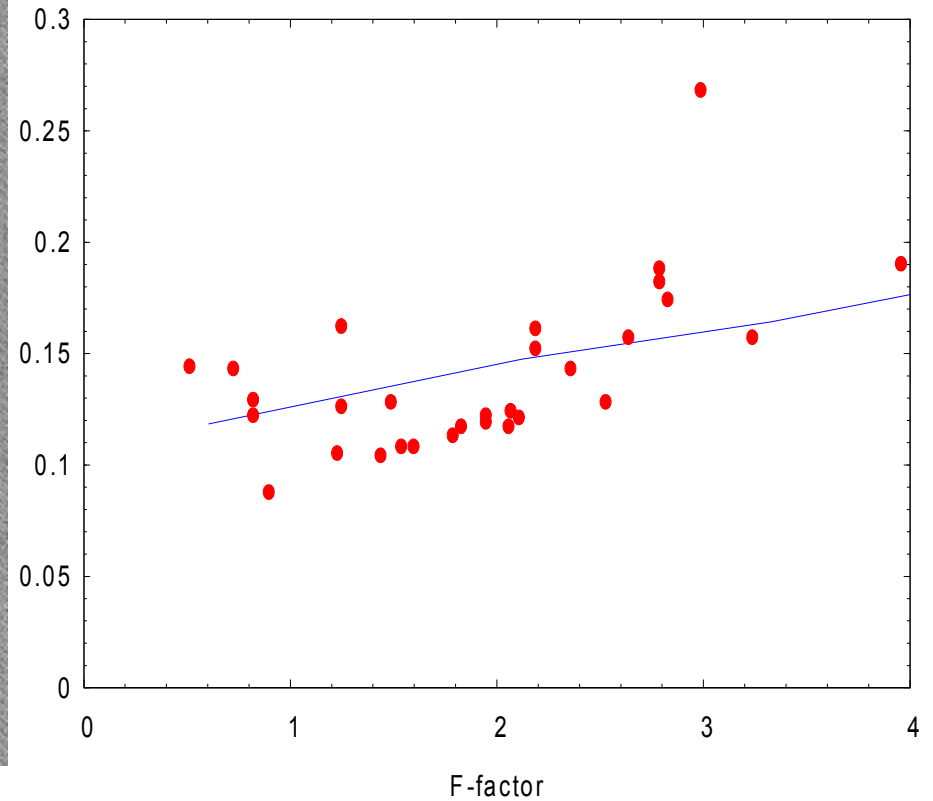
Results:

Step	Reflux liquid flow	F-factor	AHETP1	pd (mbar/m)
Units	mol/s			
1	3	1.020249	0.39489	0.132474
2	4.2	1.426565	0.382453	0.263932
3	5.4	1.832379	0.373331	0.44599
4	6.6	2.236733	0.363951	0.681693
5	7.8	2.636726	0.345768	0.972005
6	9	3.036686	0.316497	1.324427

Collecting Data



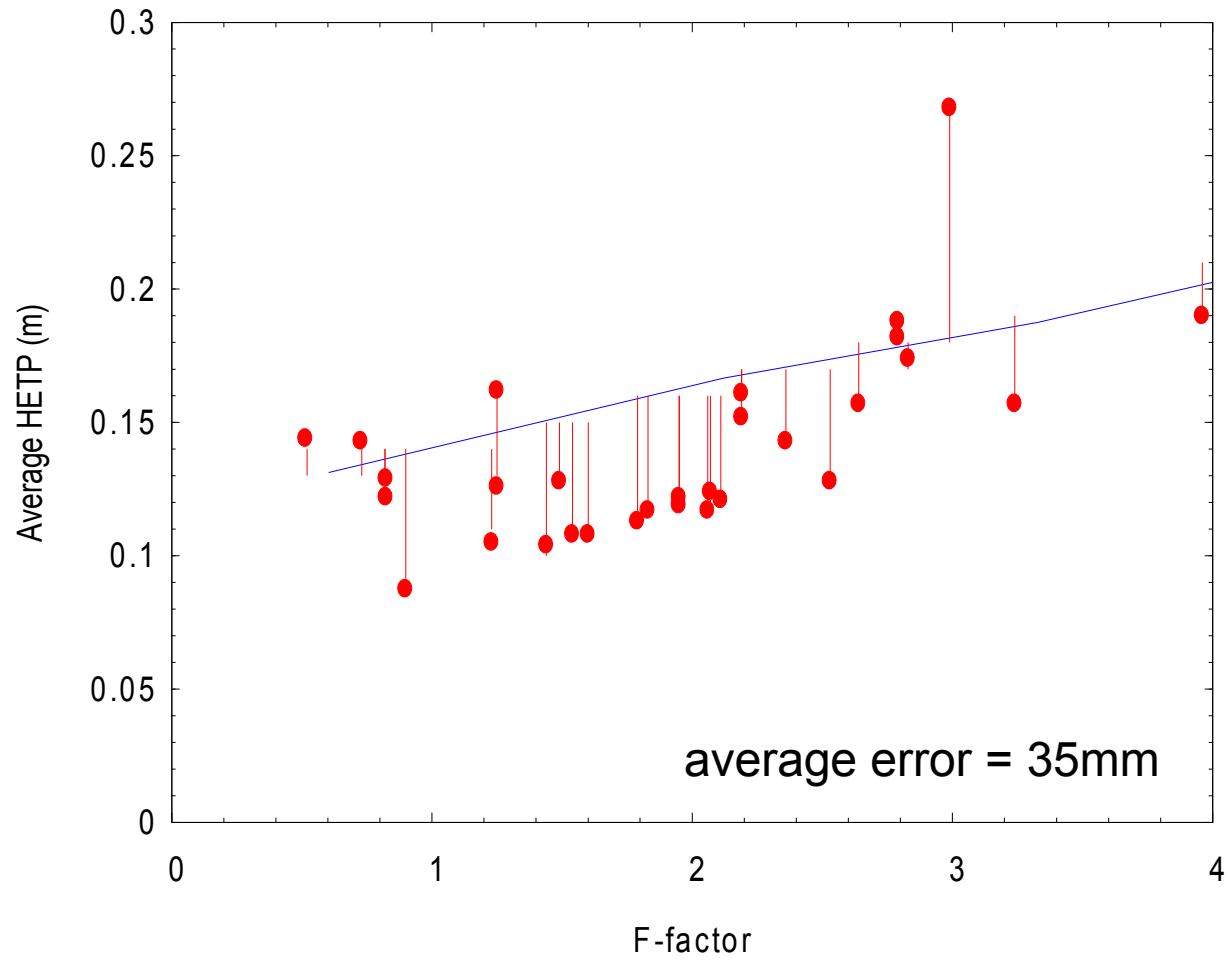
BX o/p-Xylene 16 Torr @ FRI (1.22m ID)



BRF85 — exp. ●

Model Fitness

BX o/p-Xylene 16 Torr @ FRI (1.22m ID)



BZ95 ——— exp. ● Errors ———

Structured Packing Test Data

- Sulzer Mellapak 250Y, Mellapak Plus 252Y
- Montz B1-250, B1-250M
- Koch-Glitsch Flexipac 2Y, Flexipac HC
- Raschig SuperPak 300
- Sulzer BX, BX-Plus

MTC Models

Gauze Metal Structured Packing:

- Zogg(+Toor-Marchello) 1983 [Chem.Eng.Tech., 45, p.67]
- Bravo-Fair 1985 [Hydrocarbon Processing, January]
- Brunazzi 1995 [Chem.Eng.Technol., 19, pp.20-27]
- Bravo-Rocha-Fair 1996 [IECR]

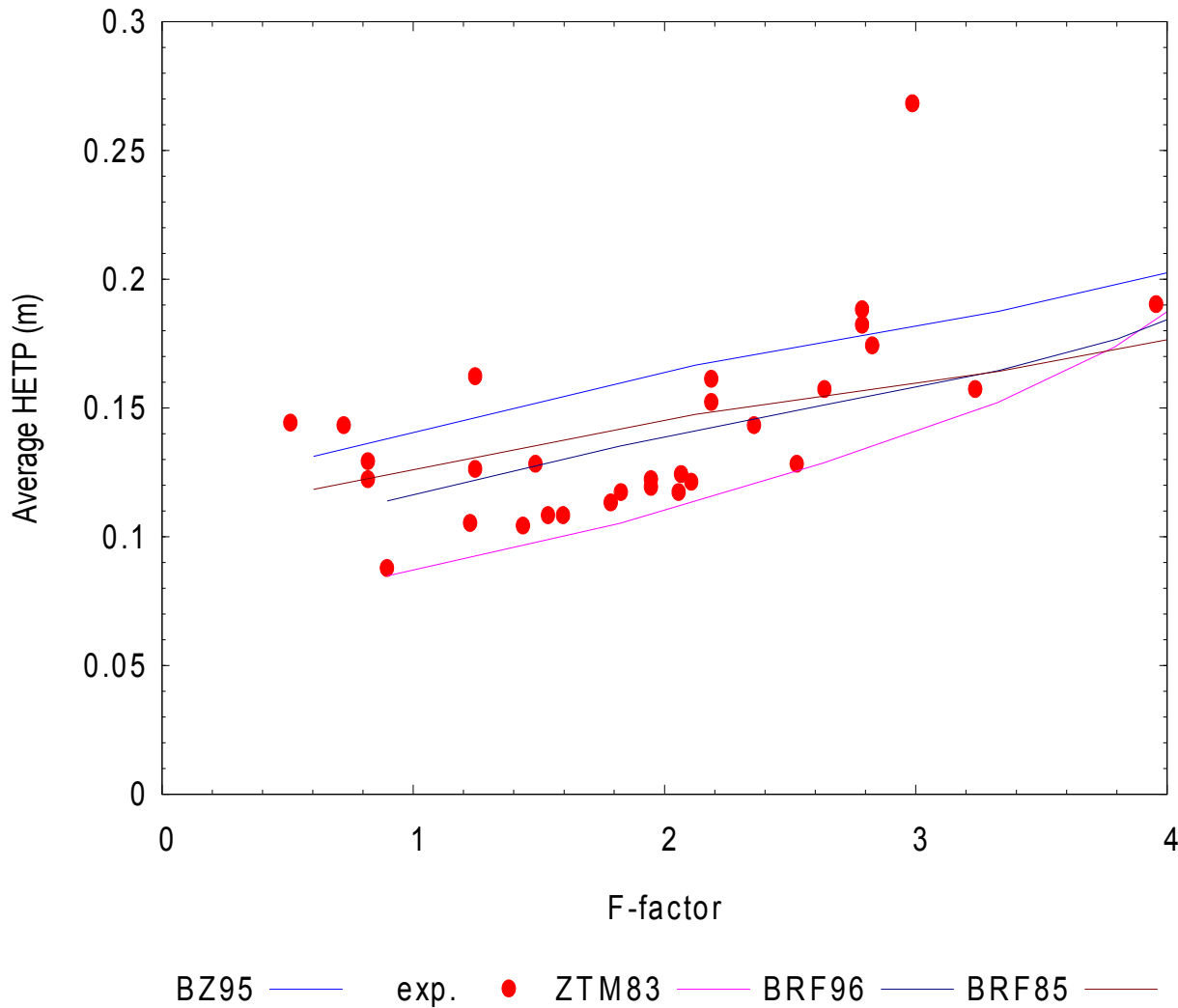
MTC Models

Sheet Metal Structured Packings:

- Bravo-Rocha-Fair 1992/1996 [DA1992, IECR]
- Billet-Schultes 1992 [Chem.Eng.Technol., 16, pp.370-375]
- Ronge 1995 [PhD]
- Olujic-Delft 1997-2003 [various]
- Erasmus-Nieuwoudt [IECR, 40, pp.2310-2321]
- Del Carlo-Olujic-Paglianti 2006 [IECR, 45, pp.7967-7976]

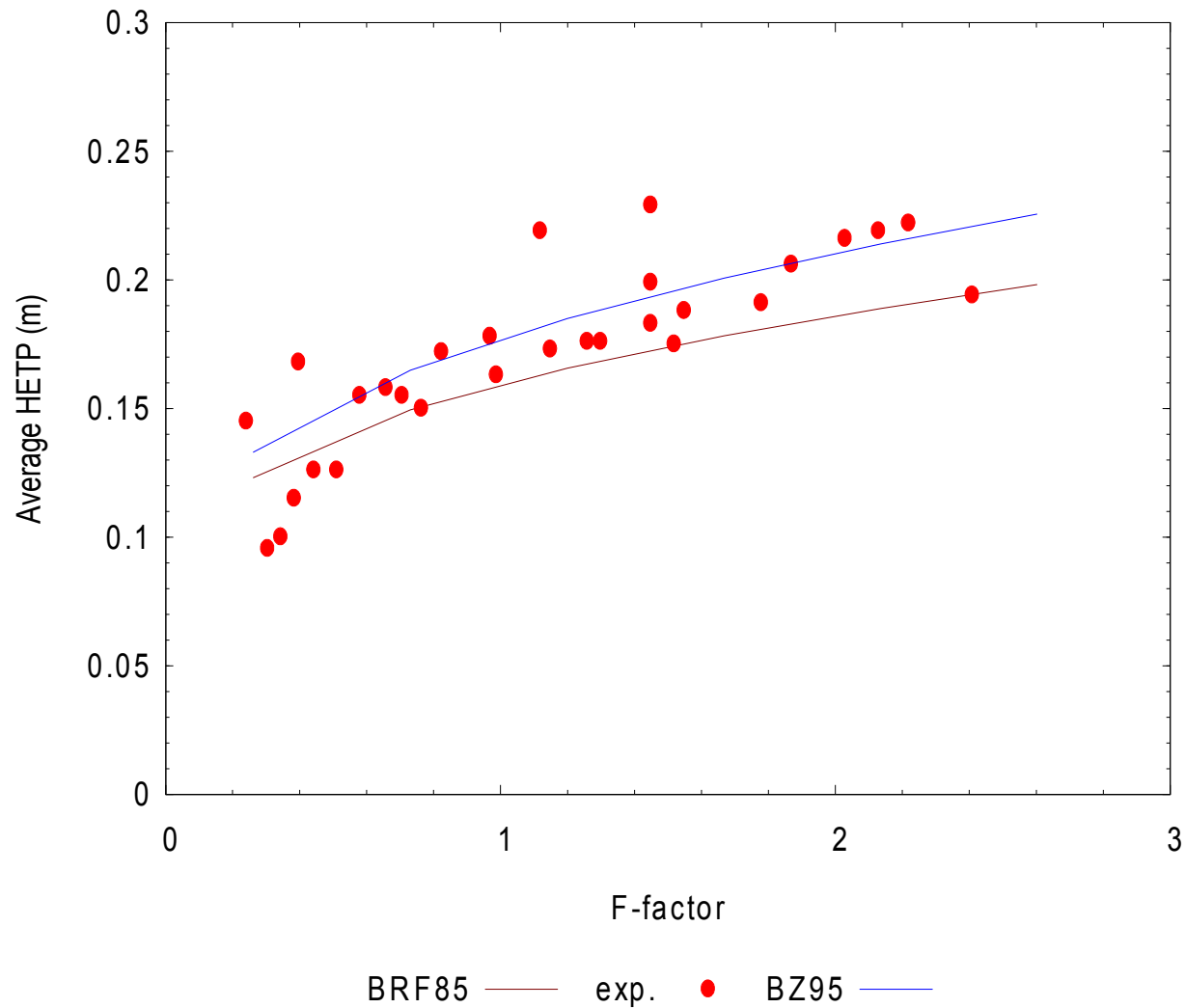
Sulzer-BX

BX o/p-Xylene 16 Torr @ FRI (1.22m ID)



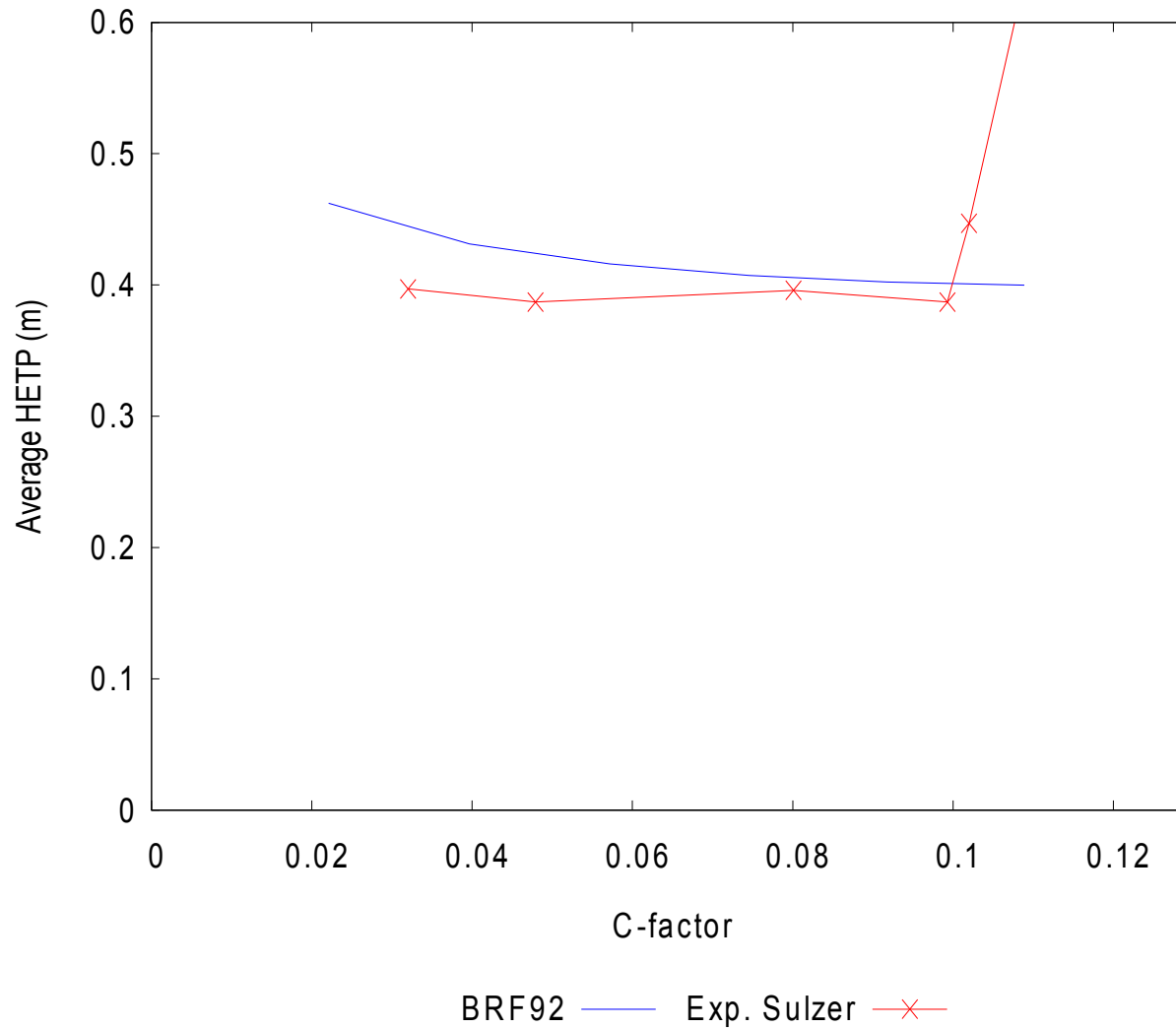
Sulzer-BX

BX o/p-Xylene 730 Torr @ FRI (1.22m ID)



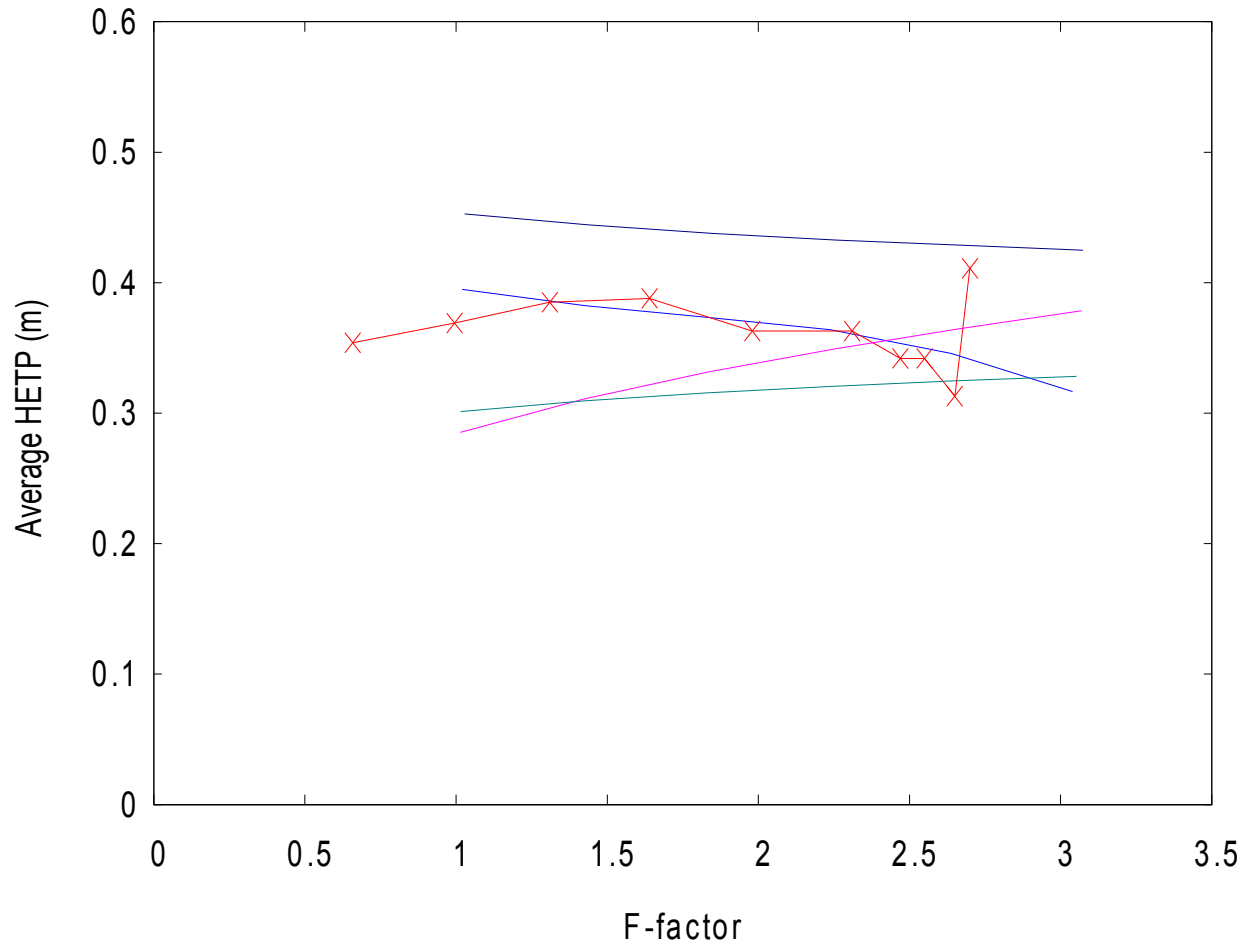
Sulzer Mellapak 250Y

M250Y CB/EB 100mbar @ Sulzer (1 ID)



Montz B1-250M

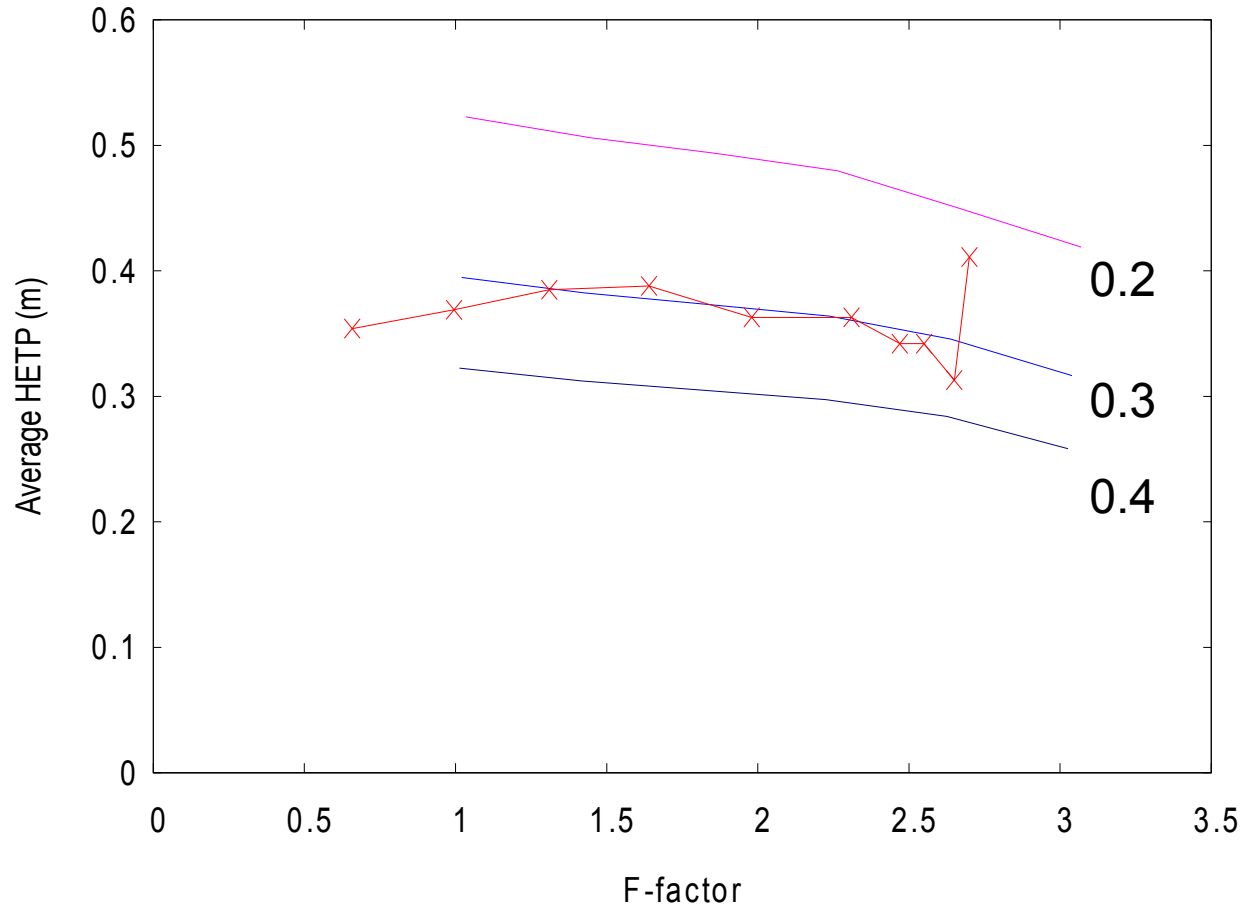
B1-250M cC6/nC7 1.03bar



BS92 — BRF85 — BRF96 —
Exp. HETP —x— BRF92 — R95 —

Billet-Schultes MTC: Effect C_V

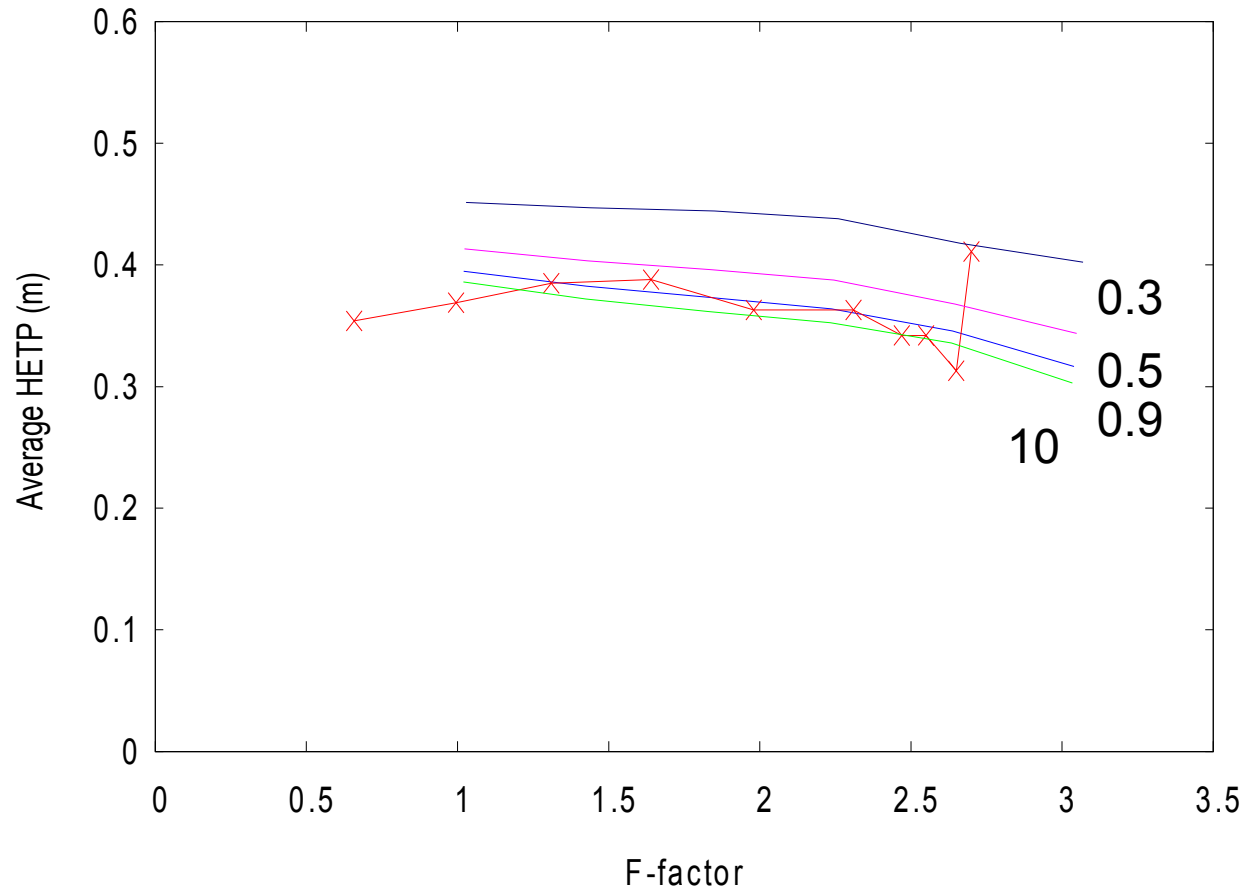
B1-250M cC6/nC7 1.03bar



BS'92 $C_V=0.3$ $Cl=0.9$ ——— BS'92 $C_V=0.2$ ———
Exp. HETP —x— BS'92 $C_V=0.4$ ———

Billet-Schultes MTC: Effect C_L

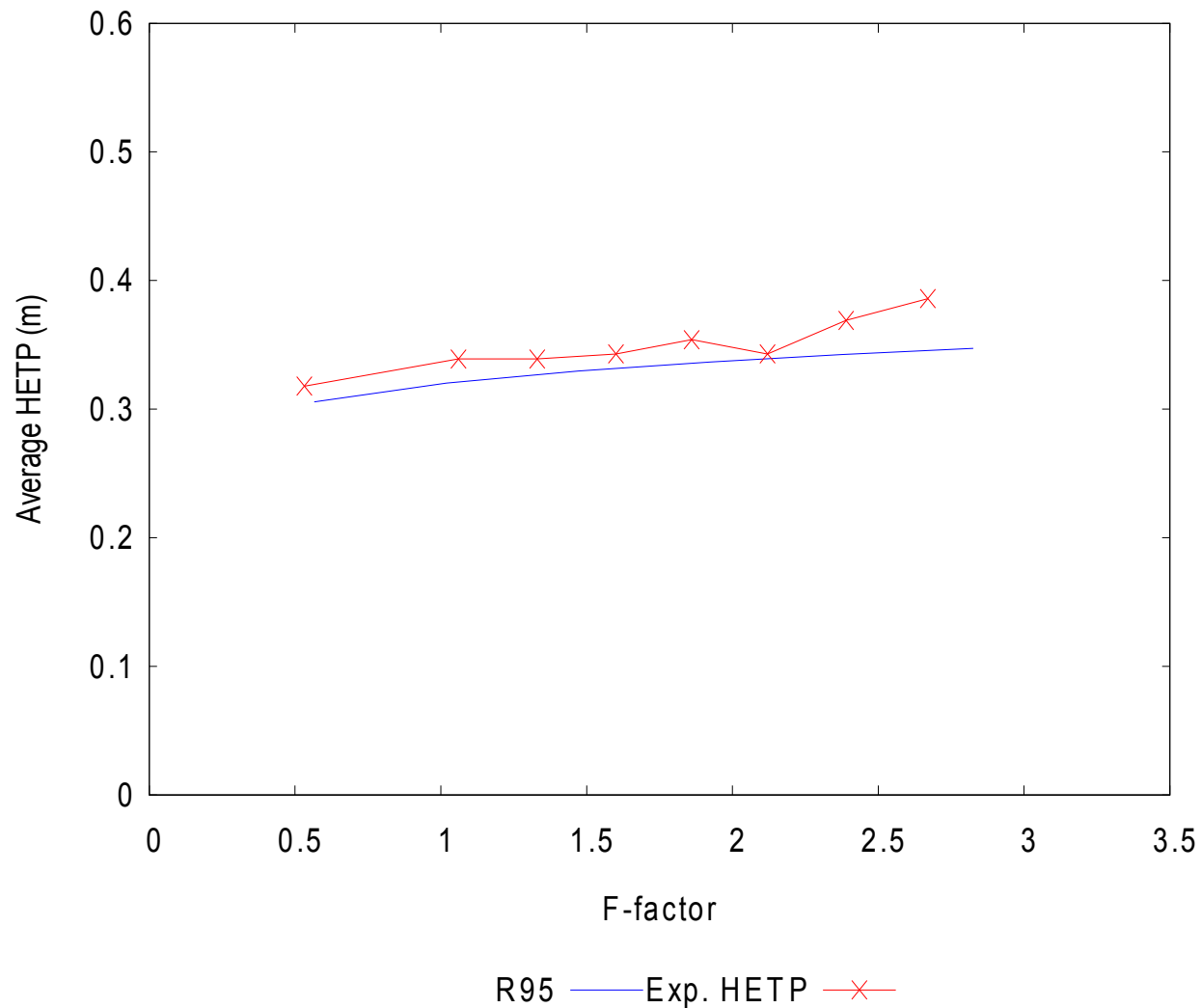
B1-250M cC6/nC7 1.03bar



BS'92 $C_v=0.3$ $C_l=0.9$ ——— BS'92 $C_v=0.3$ $C_l=0.5$ ———
 Exp. HETP —x— BS'92 $C_v=0.3$ $C_l=10.0$ ———
 BS'92 $C_v=0.3$ $C_l=0.3$ ———

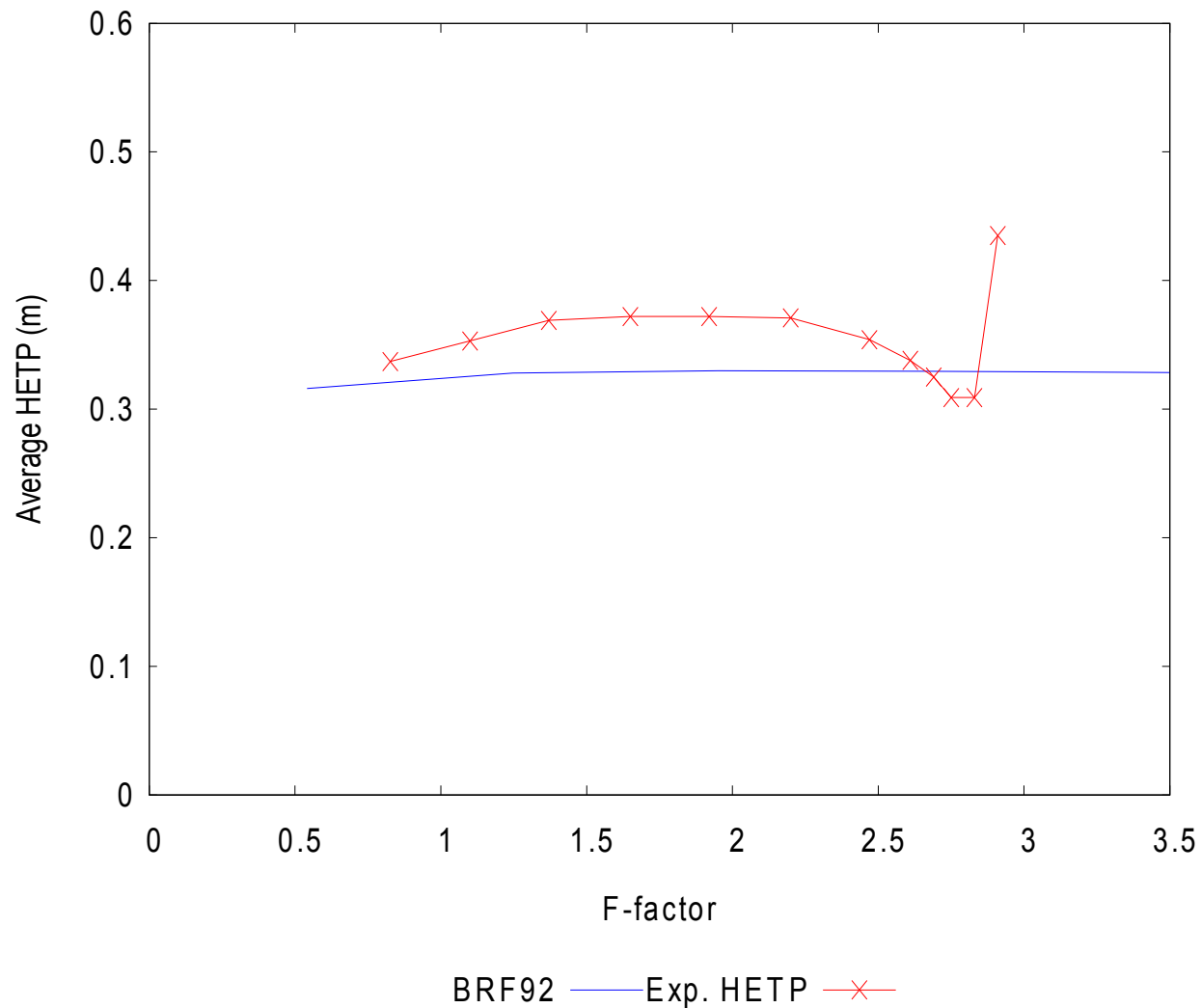
Koch-Glitsch Flexipac 2

Flexipac 2 cC6/nC7 0.33bar



Raschig SuperPak 300

SuperPak 300 cC6/nC7 1.65bar



Lack of geometry data (other than A_p): Estimated d_{eq} 30mm

EFCE WP Distillation Absorption

Conclusions

- Consistent HETP comparisons for c-C6/n-C7
- Public distillation test data collection (work in progress)
- Overall best MTC correlations (so far):
 - Gauze packings: Brunazzi '95
 - Sheet metal packings: Bravo-Rocha-Fair '92
 - New models do not provide better predictions

Future Work

- Compare pressure drop & capacity models
- Benchmark random packing models
- Model liquid entrainment @ flood in MTC?