Benchmarking Mass Transfer Correlations with a Nonequilibrium Model

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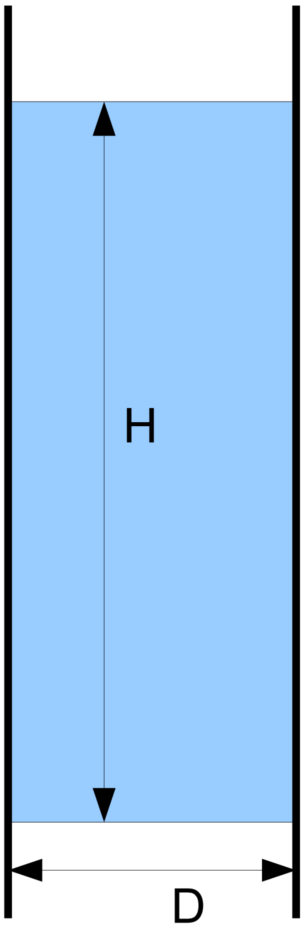
Packed Column Design

- Column Diameter:
  - Capacity: F-factor or C-factor
  - Pressure Drop: HETP/Δp
- 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

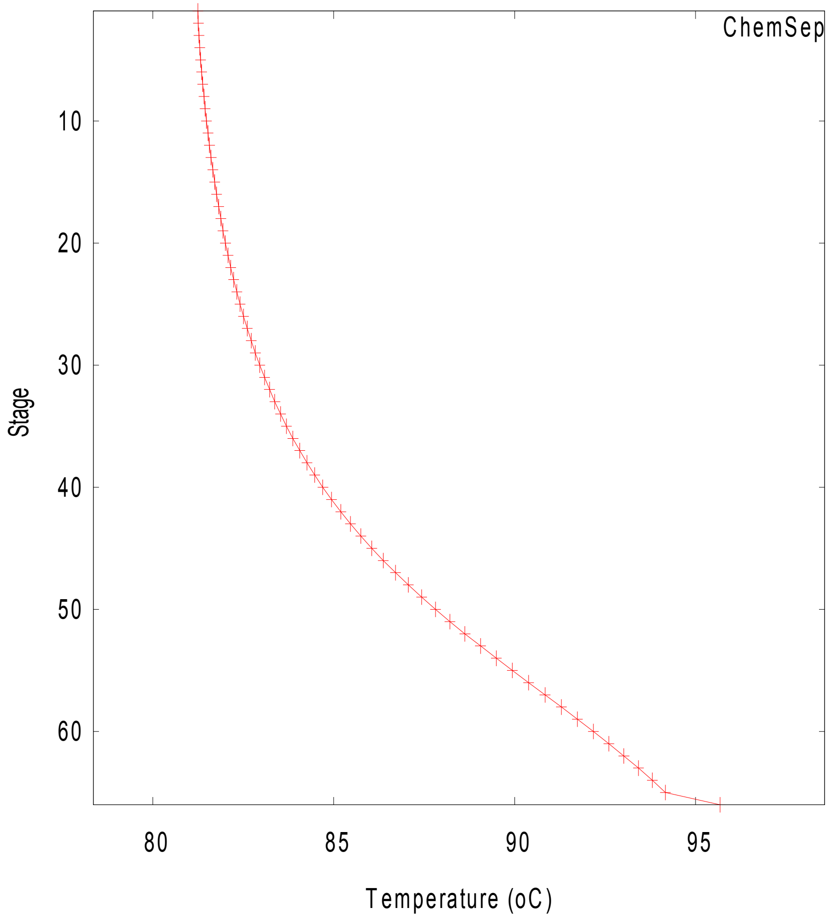
How constant is the HETP?

HETP vs. Packed Bed Height

HETP varies due to:

- T & p changes

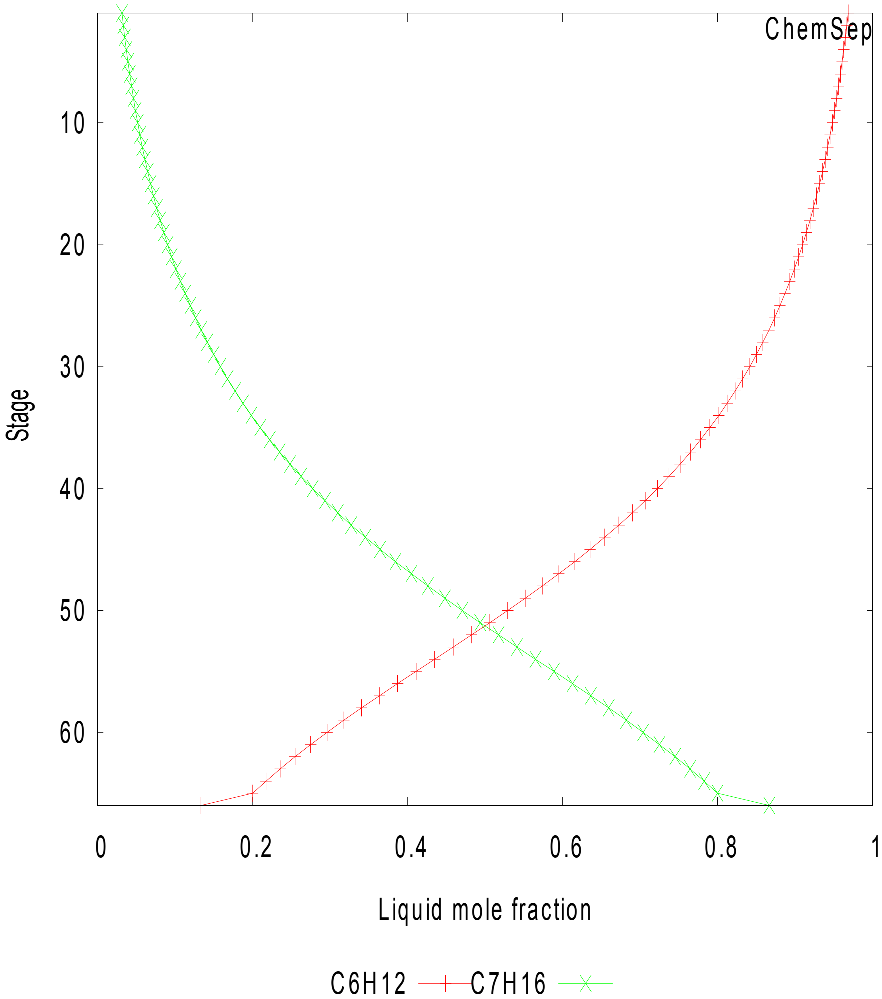
c-C6/n-C7 1atm, 3m bed



HETP vs. Packed Bed Height

HETP varies due to:

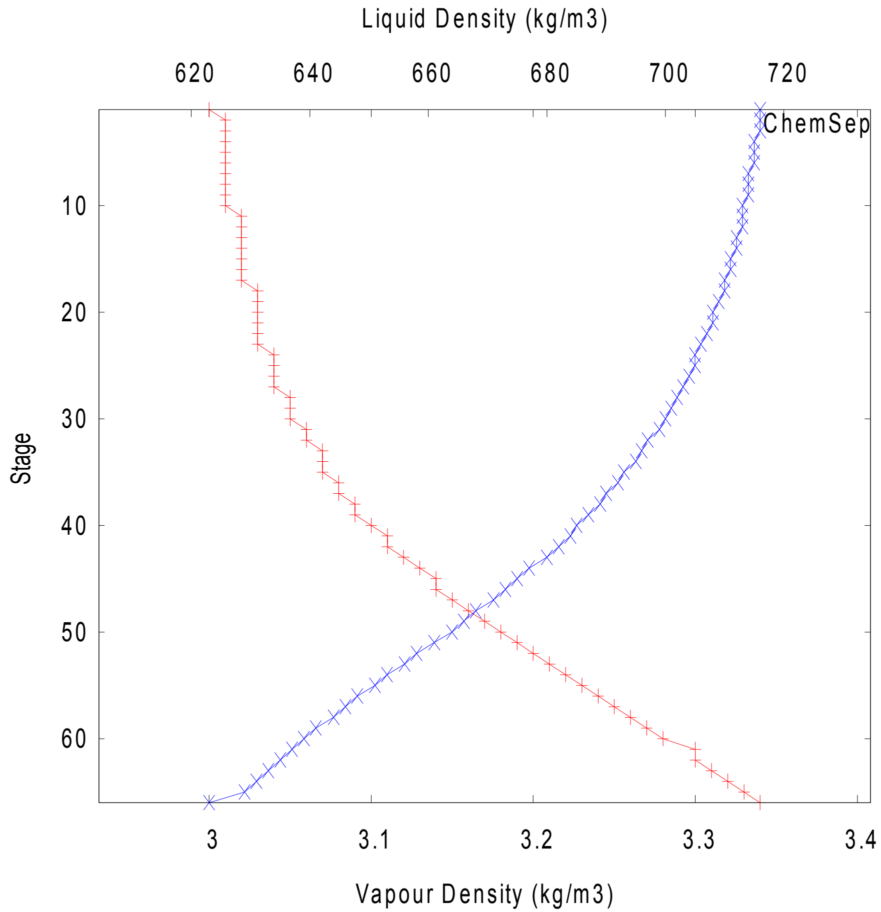
- T & p changes
- Concentration changes



HETP vs. Packed Bed Height

HETP varies due to:

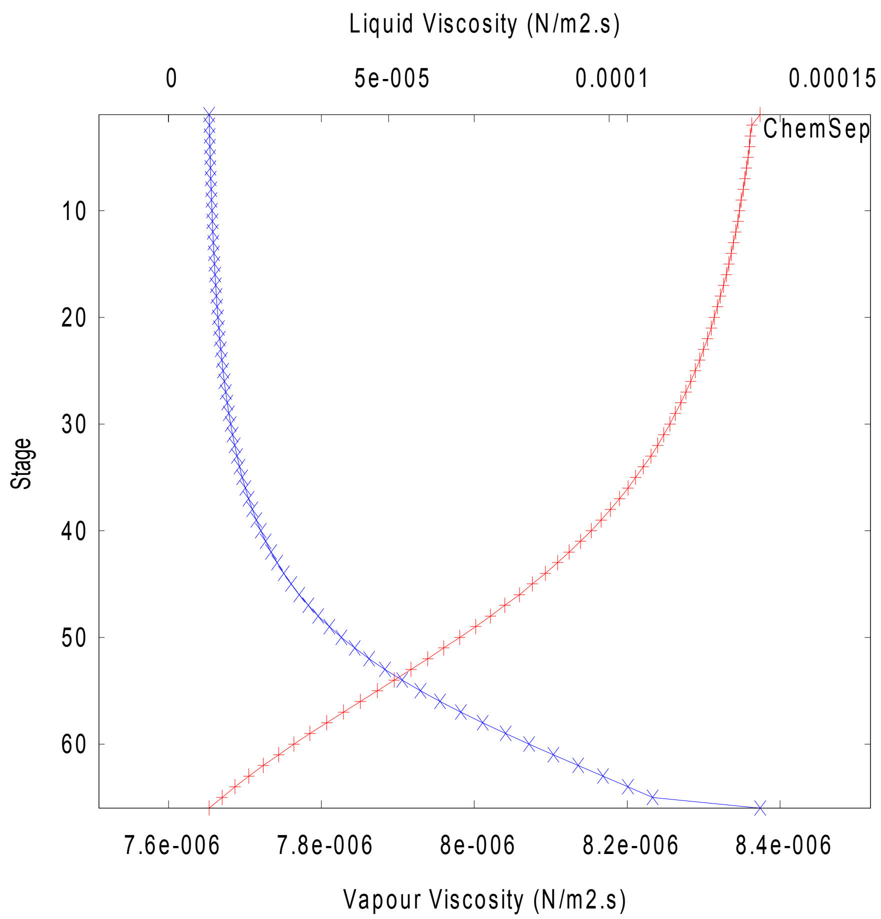
- T & p changes
- Concentration changes
- Consequent changes in densities



HETP vs. Packed Bed Height

HETP varies due to:

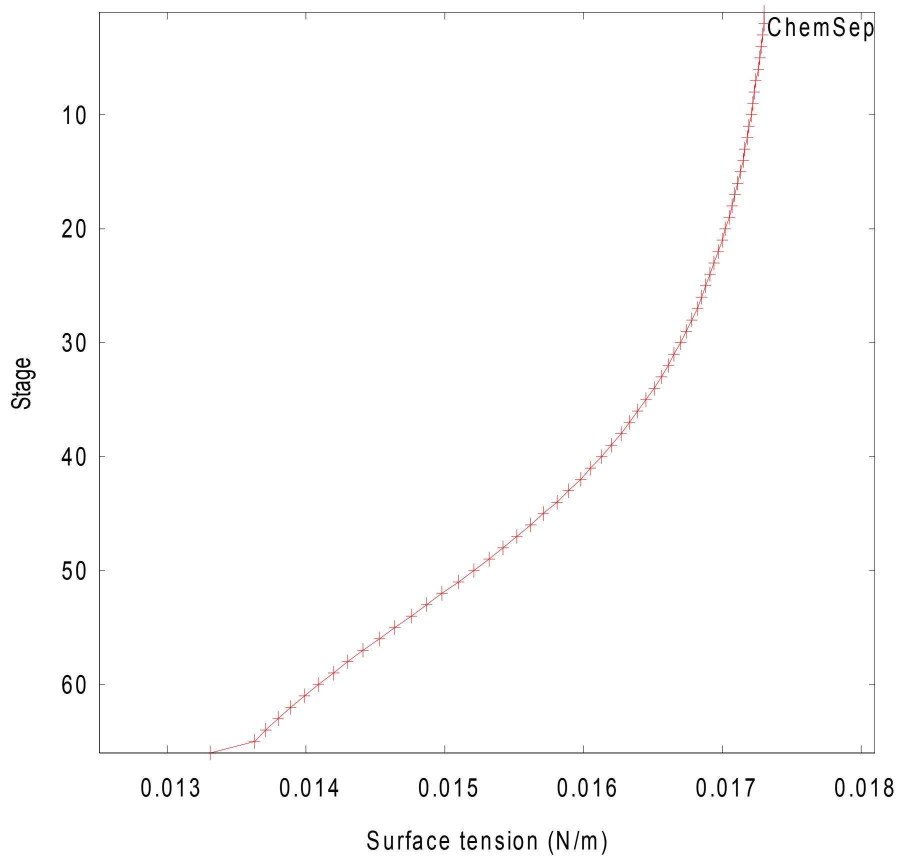
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities



HETP vs. Packed Bed Height

HETP varies due to:

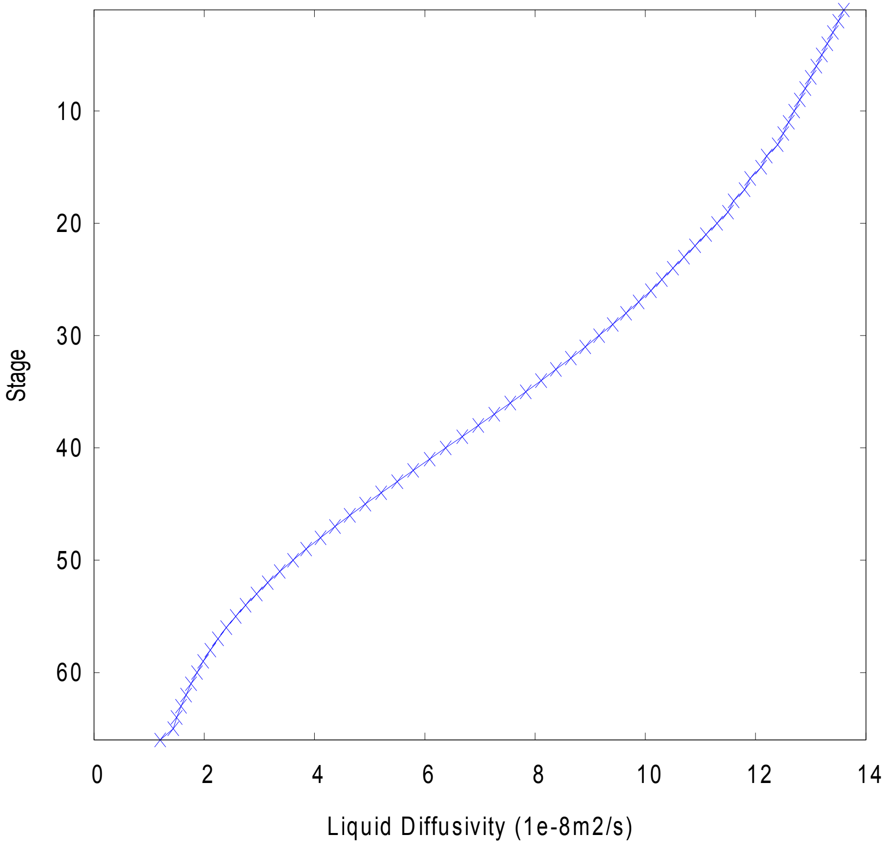
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension



HETP vs. Packed Bed Height

HETP varies due to:

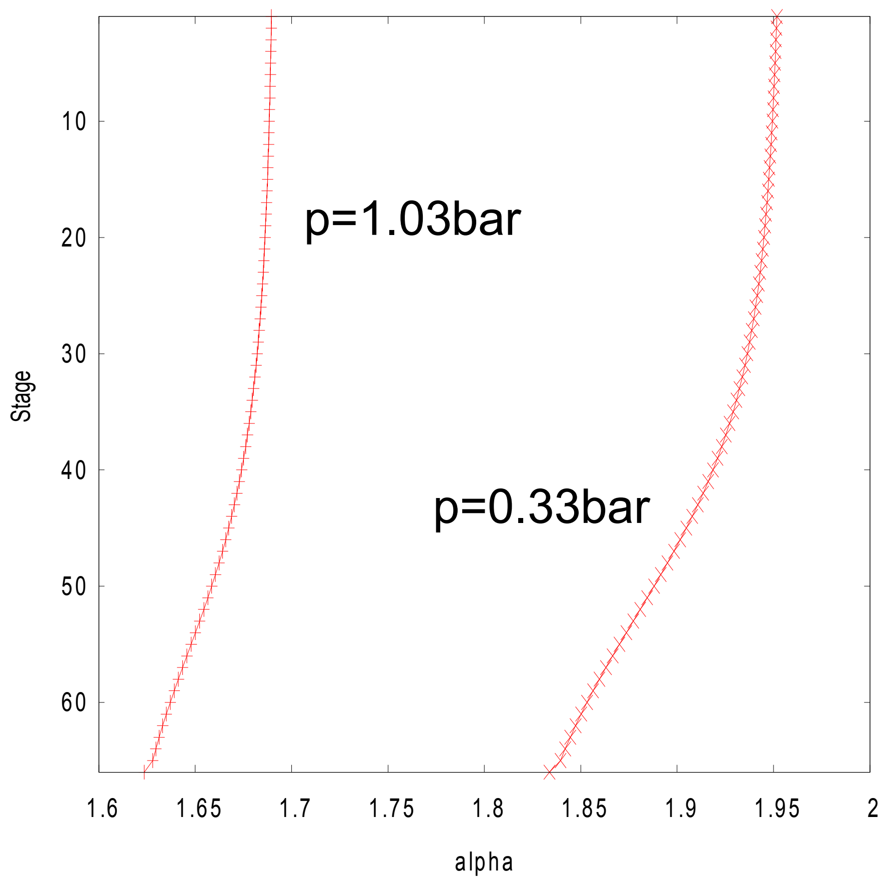
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities



HETP vs. Packed Bed Height

HETP varies due to:

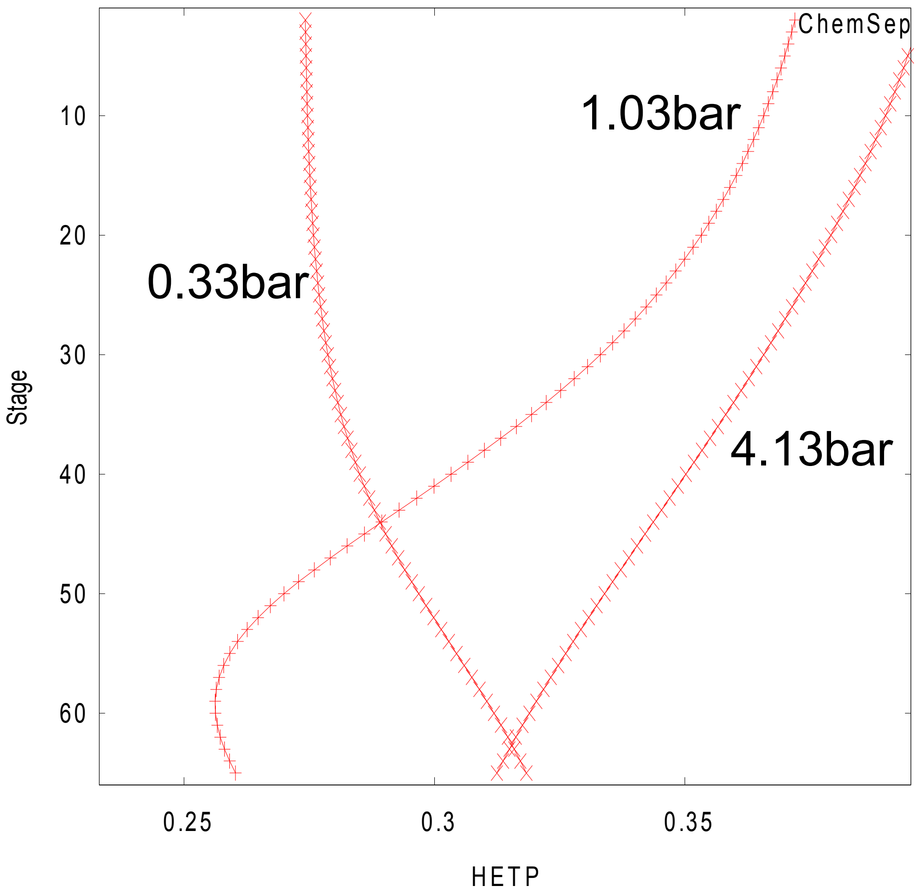
- T & p changes
- Concentration changes
- Consequent changes in densities, viscosities, surface tension, and diffusivities
- And changes in relative volatility



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
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- Consequent changes in densities, viscosities, surface tension, and diffusivities
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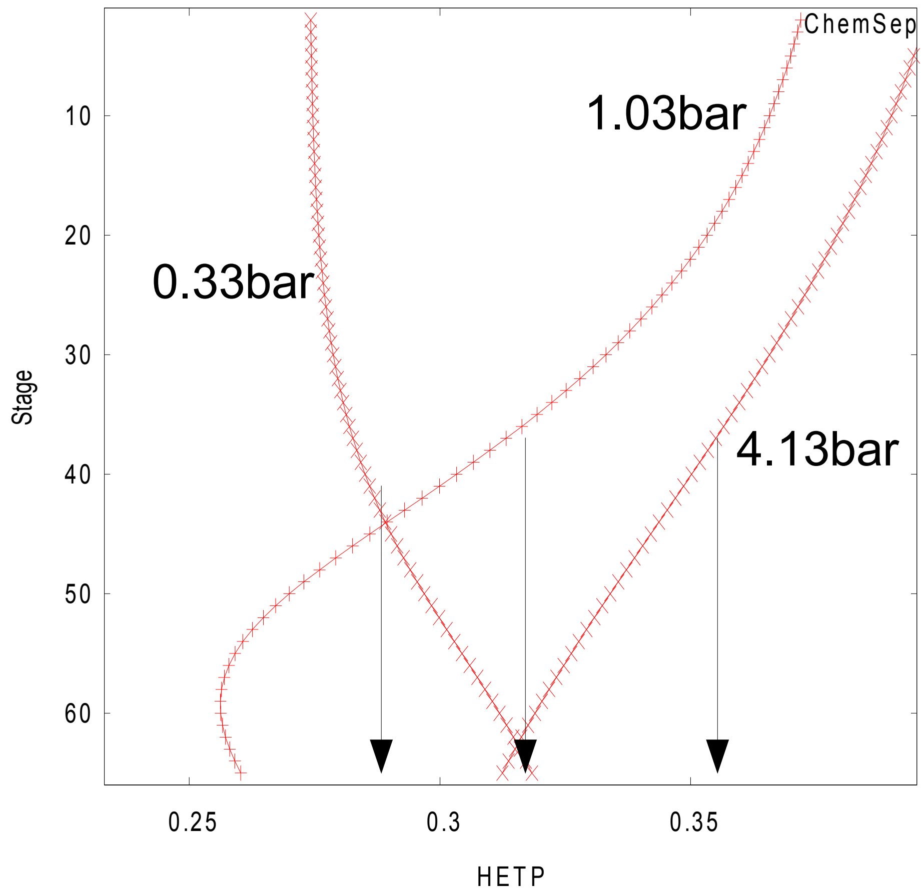


We must average HETP over the bed height!

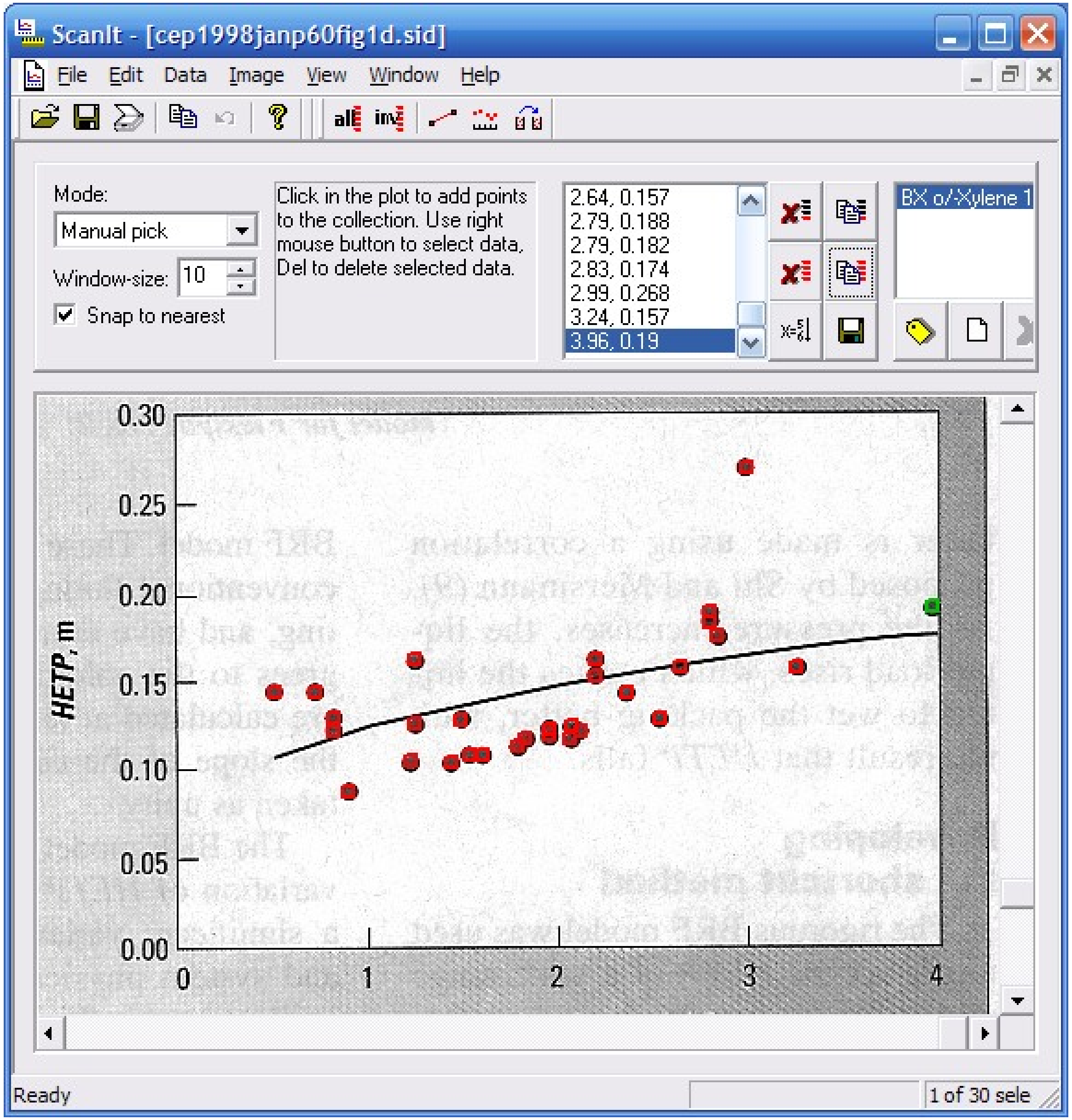
A Different Approach

- 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

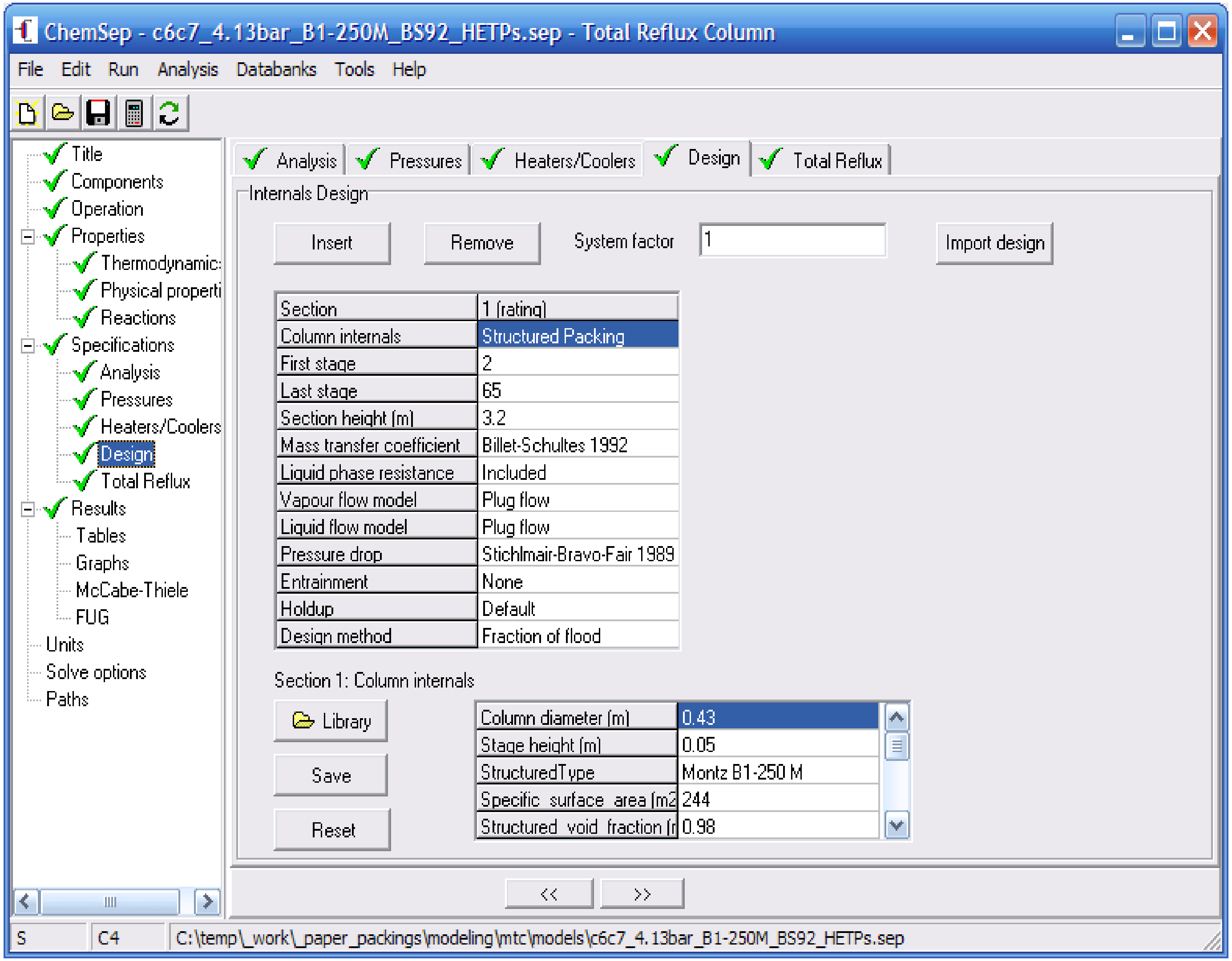
Collecting Data

- “ScanIt”



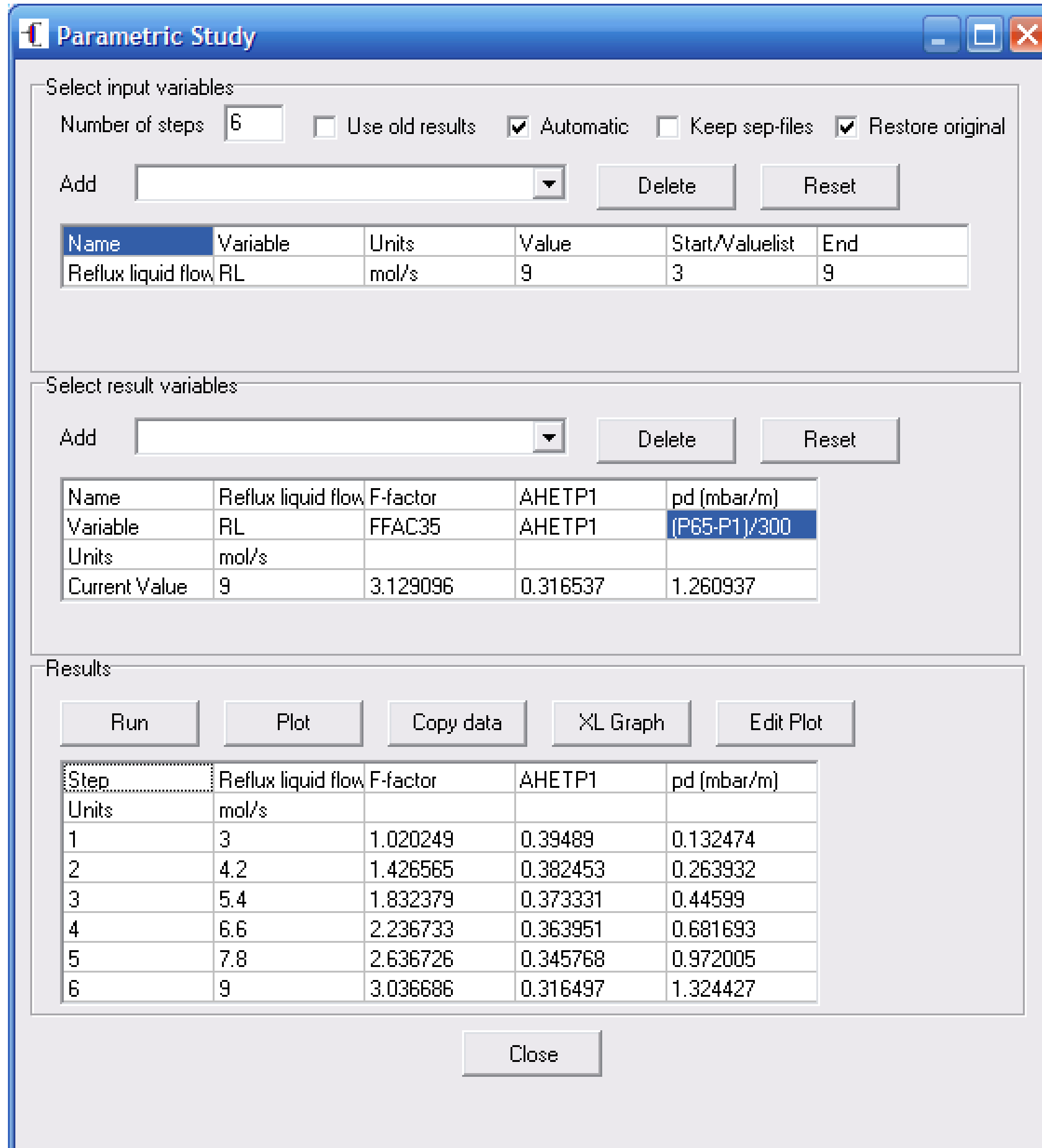
Collecting Data

- "ScanIt"
- Simulate it: ChemSep Total Reflux

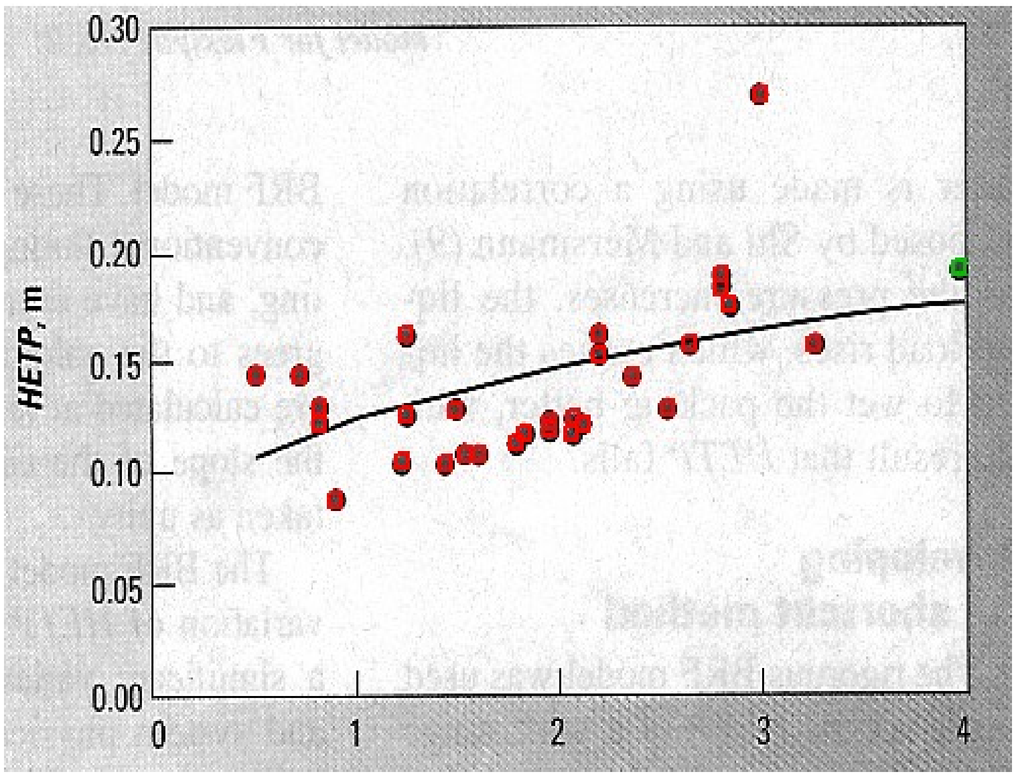


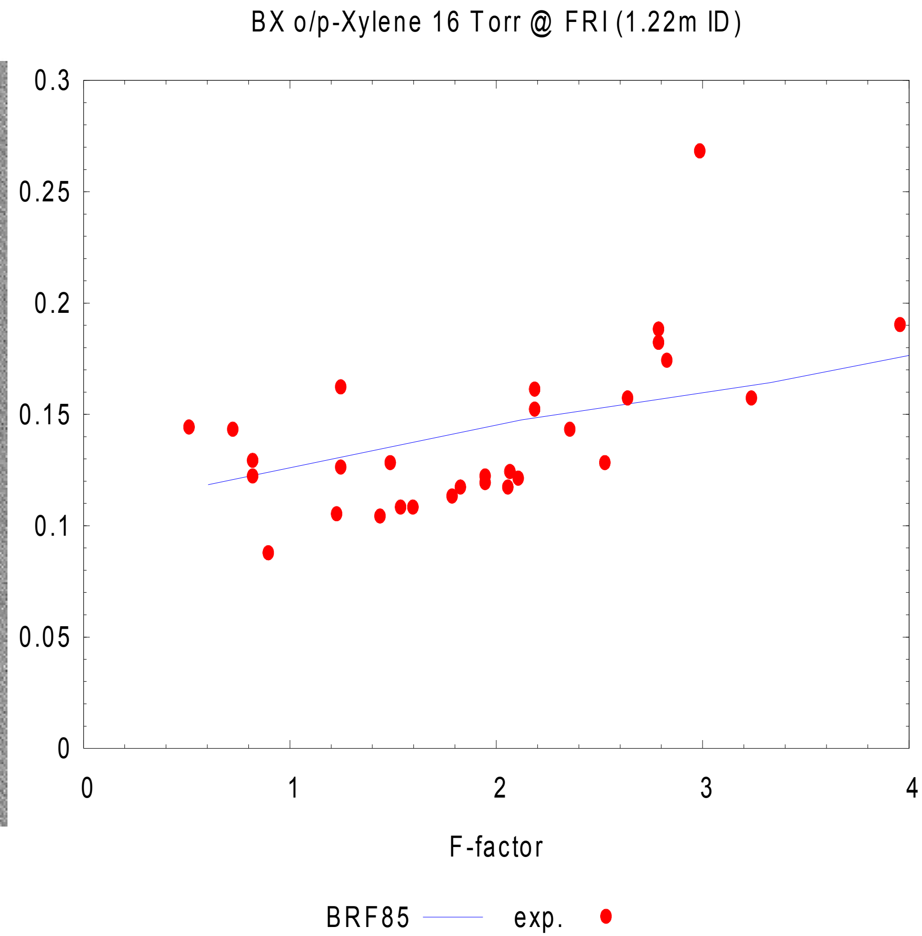
Collecting Data

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

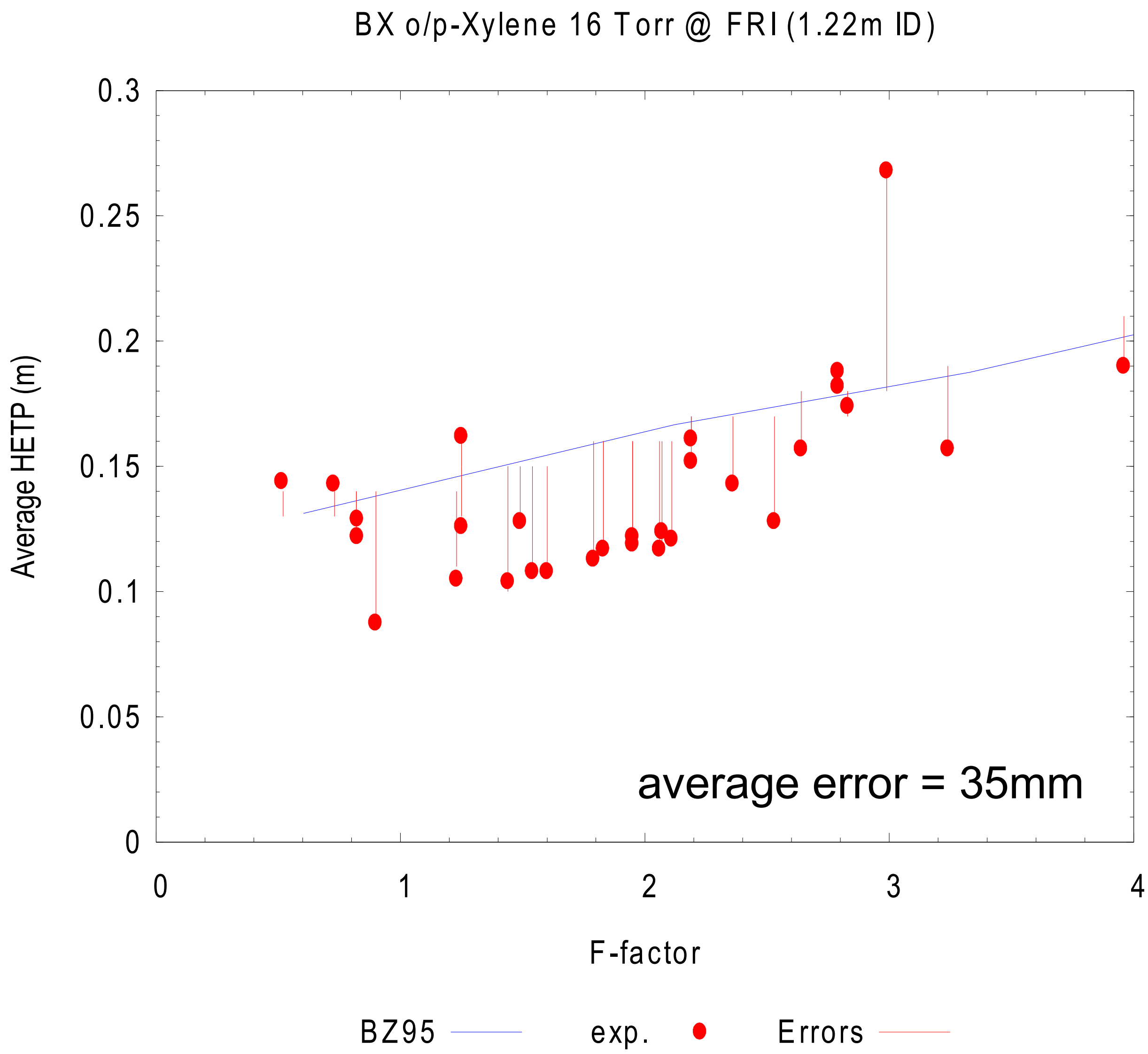


Collecting Data





Model Fitness



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:

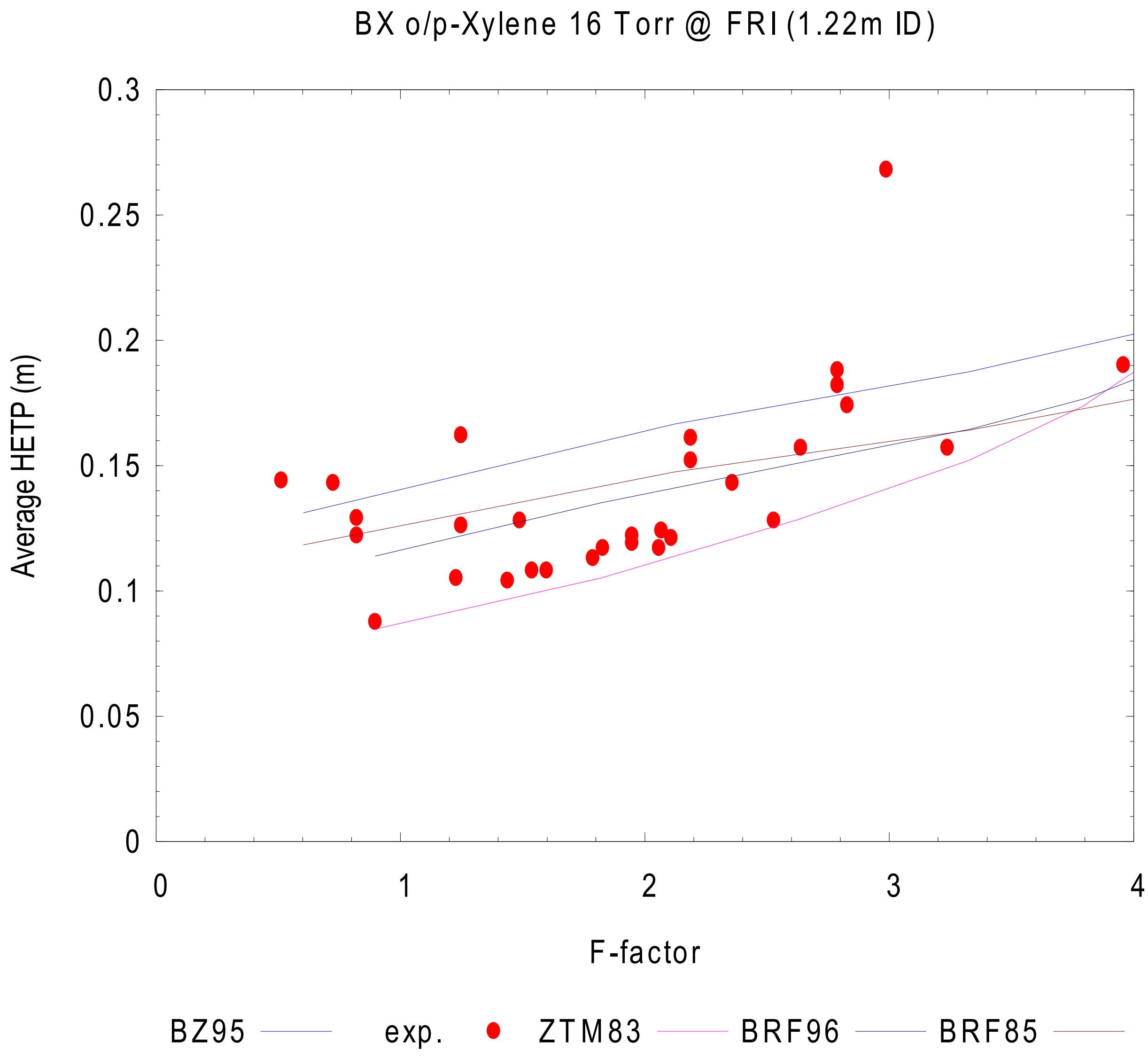
- Zogg(+Toor-Marchello) 1983 [Chem.Ing.Tech., 45, p.67]
- Bravo-Fair 1985 [Hydrocarbon Processing, January]
- Brunazzi 1995 [Chem.Eng.Technol., 19, pp.20-27]
- Bravo-Rocha-Fair 1996 [IECR]

MTC Models

Sheet Metal Structured Packings:

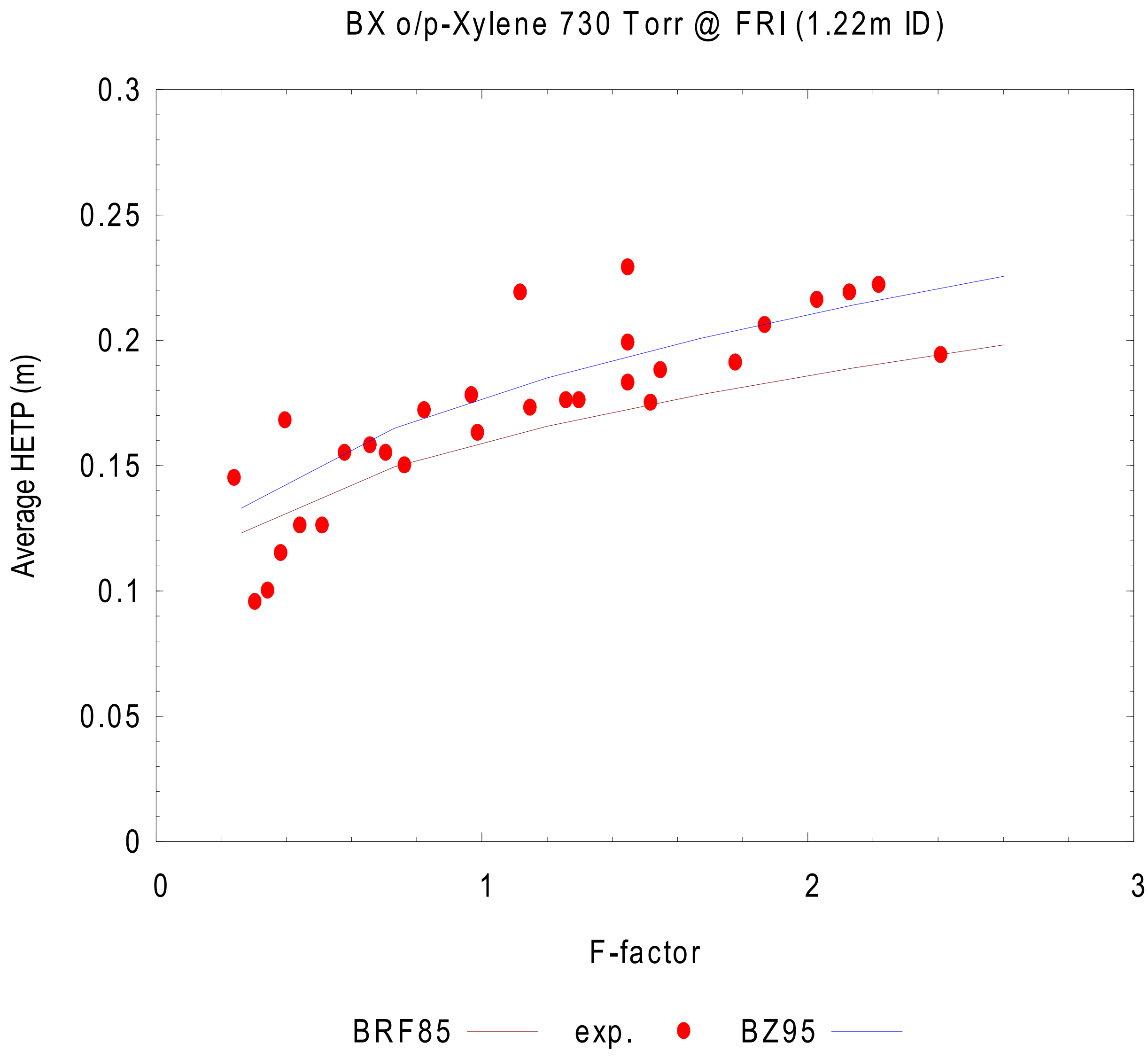
- Bravo-Rocha-Fair 1992/1996 [DA1992, IECR]
- Billet-Schultes 1992 [Chem.Eng.Technol., 16, pp.370-375]
- Ronge 1995 [PhD]
- Olujic-Delft 1997-2003 [various]
- Erasmus-Nieuwoudt [IECR, 40, pp.2310-2321]
- Del Carlo-Olujic-Paglianti 2006 [IECR, 45, pp.7967-7976]

Sulzer-BX



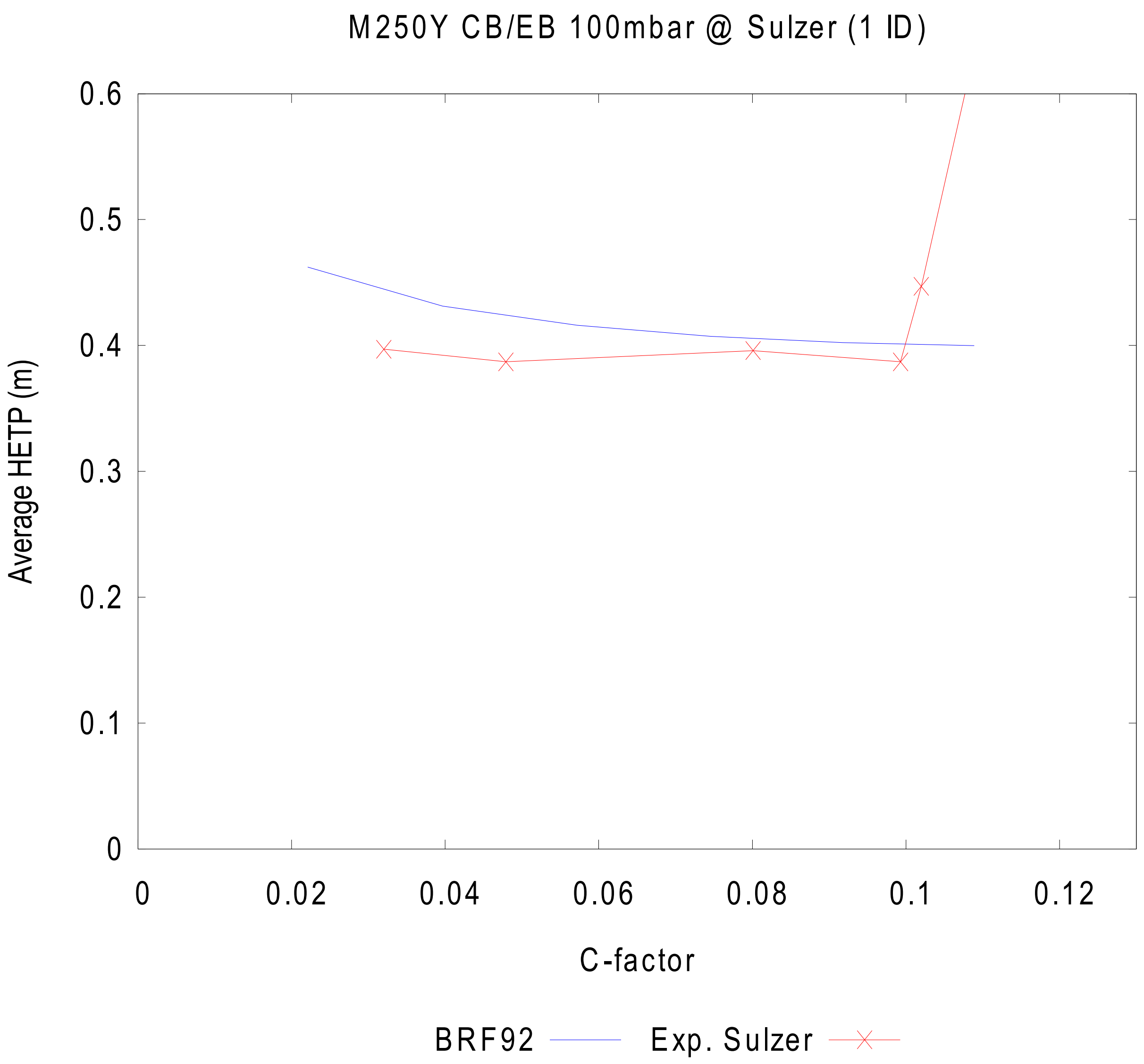
BX o/p-Xylene 16 Torr @ FRI (1.22m ID)
0.3
0.25
0.2
0.15
0.1
0.05
0
Average HETP (m)
0
1
2
3
4
F-factor
BZ95
exp.
ZTM83
BRF96
BRF85

Sulzer-BX

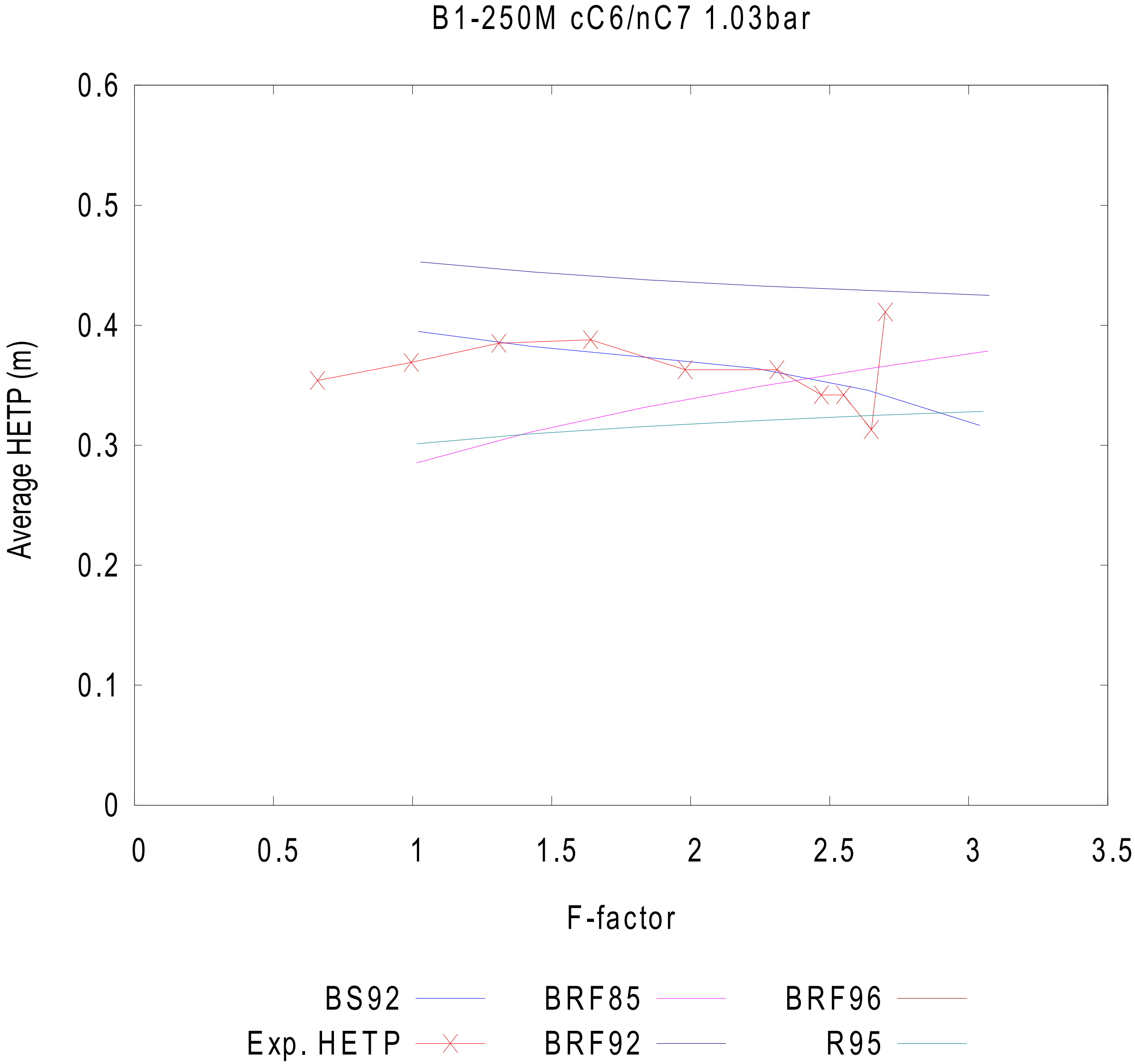


BX o/p-Xylene 730 Torr @ FRI (1.22m ID)
Average HETP (m)
0.3
0.25
0.2
0.15
0.1
0.05
0
0
1
2
3
F-factor
BRF85
exp.
BZ95

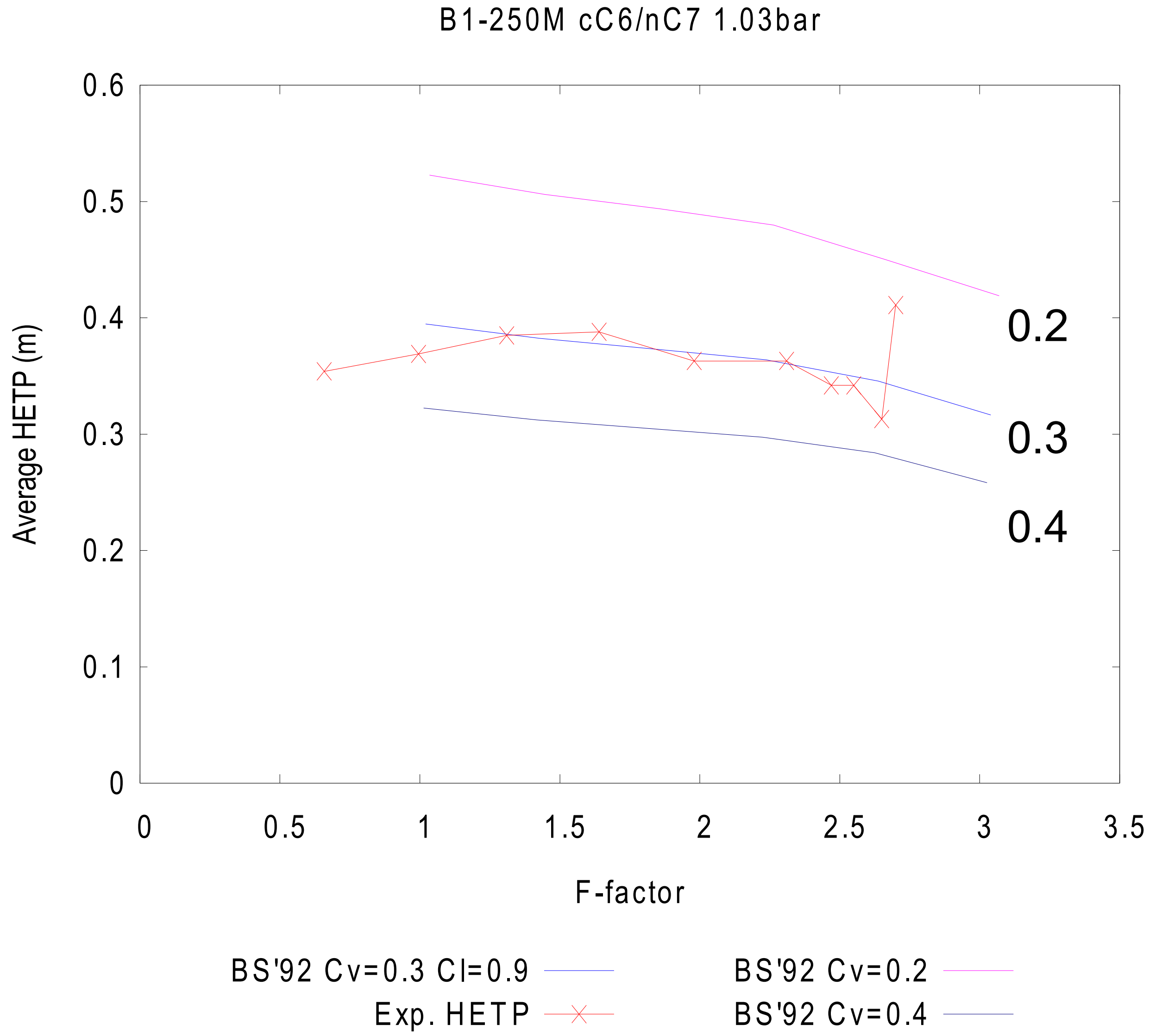
Sulzer Mellapak 250Y



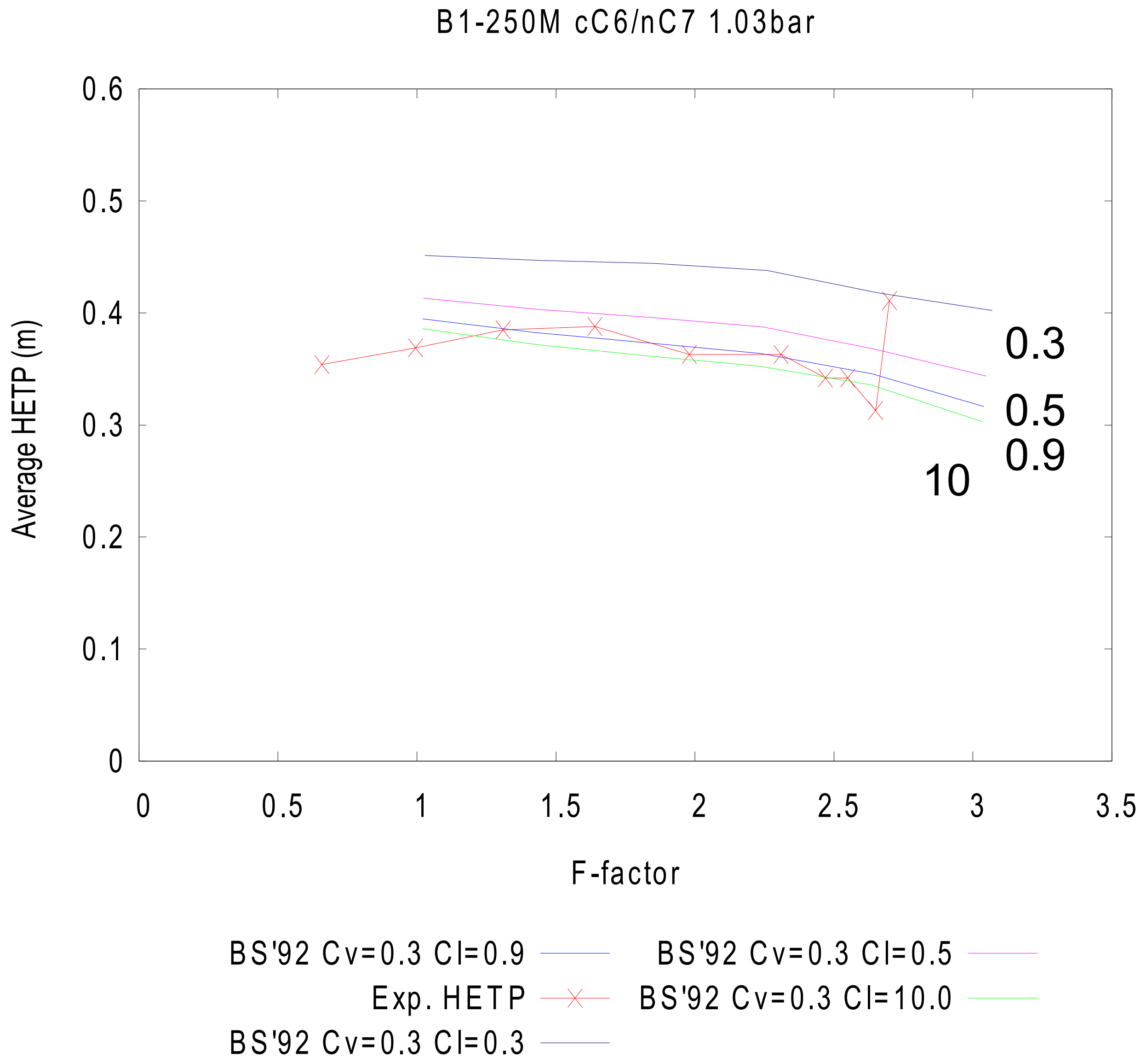
Montz B1-250M



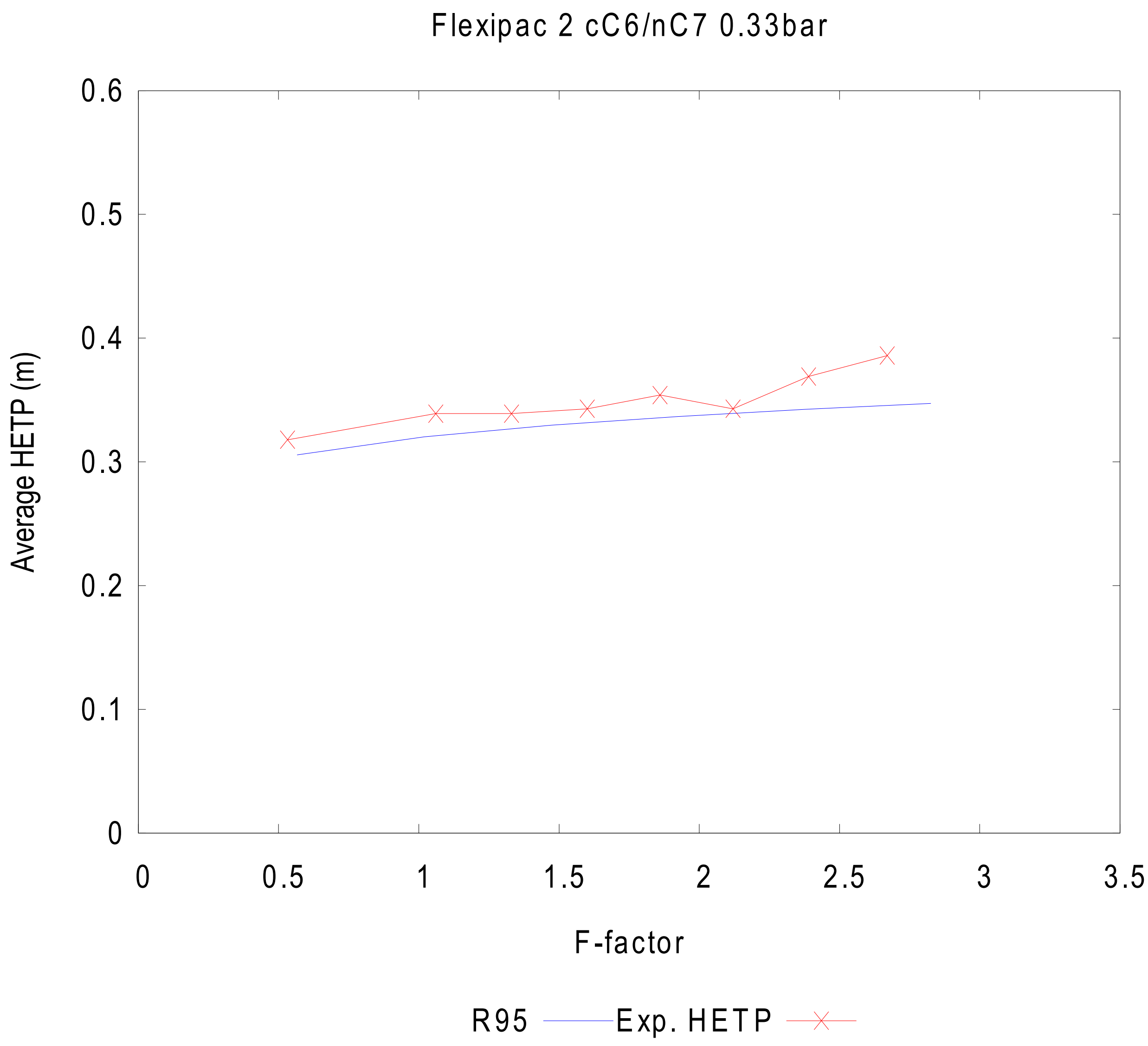
Billet-Schultes MTC: Effect C_V



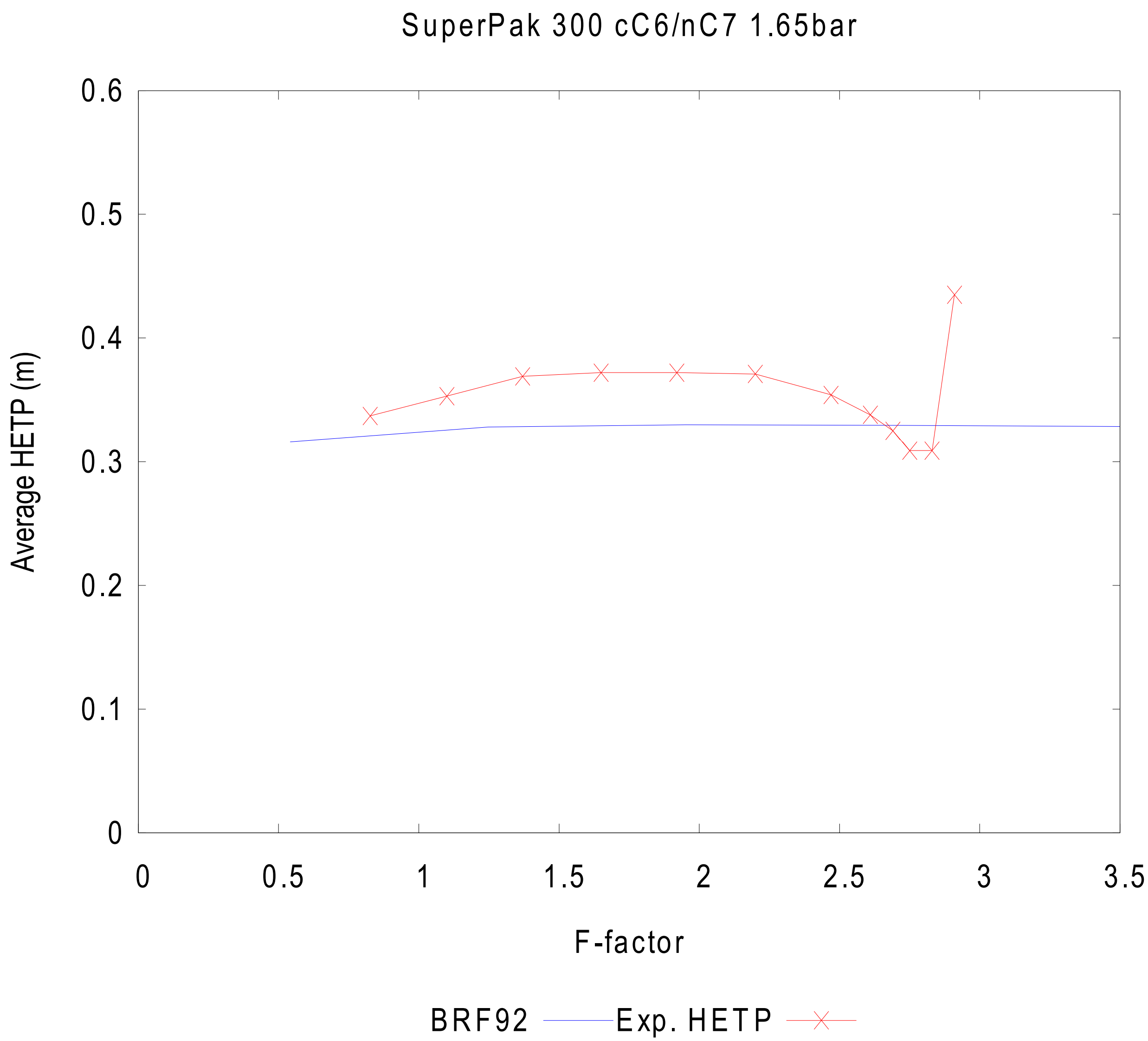
Billet-Schultes MTC: Effect C_L



Koch-Glitsch Flexipac 2



Raschig SuperPak 300



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

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?