WHITE PAPER

Column Analysis in Aspen Plus® and Aspen HYSYS®: Validation with Experimental and Plant Data

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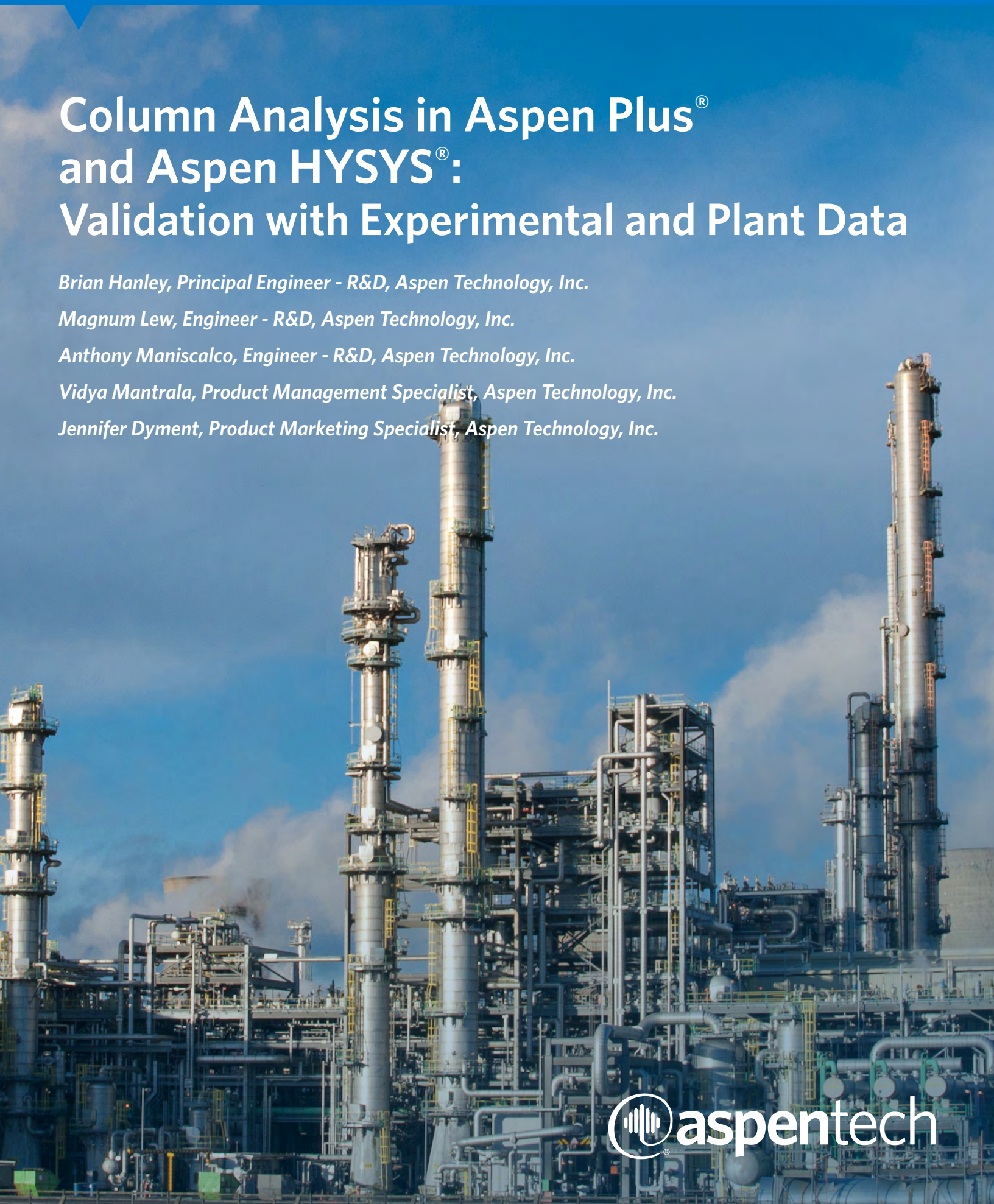

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Introduction

Predicting the hydraulic performance of trays and packing is a critical component in the simulation of towers for process design, process performance and process reconciliation purposes. The hydraulic limitations on these types of internals define acceptable operating envelopes for towers or tower sections. In addition to the predictions about limiting vapor and liquid flows, the hydraulic predictions tie the pressure drop and mass-transfer efficiencies of the internals to the vapor and liquid traffic in the column. The pressure, at any point in the column, is directly related to the relative volatilities of the components in the mixture, so it is clear that equipment pressure drop predictions (including the contribution of the static vapor head) need to be as accurate as possible. In addition, the internal vapor and liquid traffic imposes certain separation efficiency limitations on the internals; for example, as the maximum useful capacity for both trays and packing is approached, the separation efficiency will plateau.

With the new Column Analysis feature in V9 of Aspen Plus® and Aspen HYSYS®, the underlying code related to tray and packing hydraulics has been extensively reviewed and updated. A greater range of tabulated results are now available which are in much closer agreement to experiments and to industry-standard design/rating software such as KG-TOWER® (publically available from the vendor Koch-Glitch) and Sulcol™ (publically available from the vendor Sulzer ChemTech).

This white paper compares the results from new functionality, shared in both Aspen Plus and Aspen HYSYS, to KG-TOWER and Sulcol software, as well as with experimental data.

In addition to improving the underlying code related to tray and packing hydraulics, a new, interactive column visualization tool has been added in both Aspen HYSYS and Aspen Plus. Figure 1 shows the new user interface, which has been tested with engineers working on design or operations at 30 top companies.

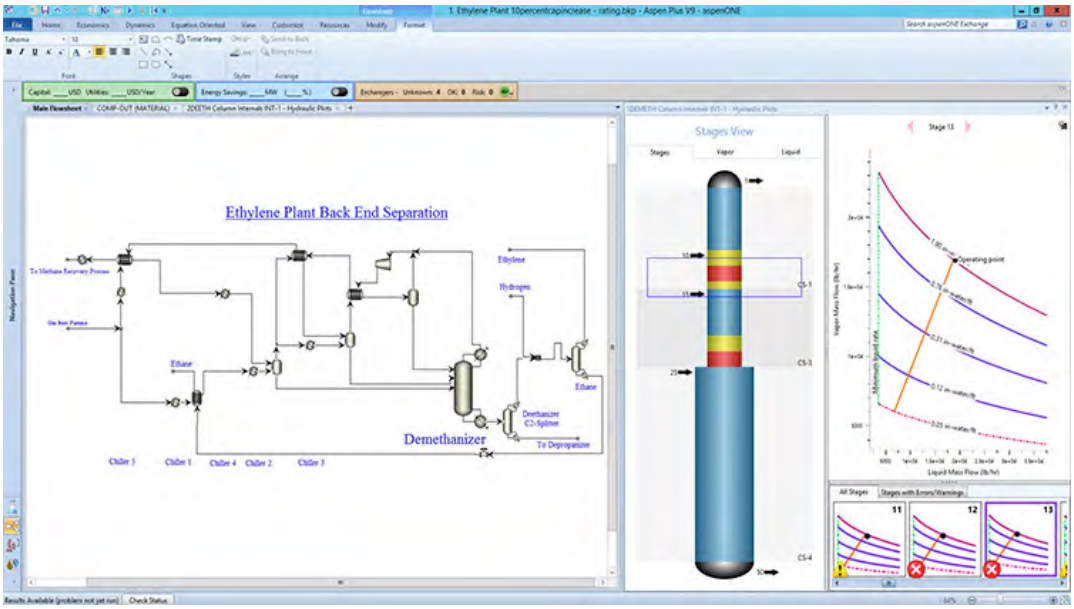

Figure 1: The new user interface for the Column Analysis feature in Aspen Plus allows for eased analysis workflows. The feature looks and acts identically in Aspen Plus.

The improvements to the Column Analysis workflow can be found in the in-product documentation (F1 help) available inside Aspen Plus and Aspen HYSYS.

Improvements to Tray Hydraulic Correlations

The correlations for the standard, cross-flow tray types in the Aspen Technology tray database have been improved to better fit both the literature models, as well as published data from FRI experiments. The results are detailed below, along with references.

Samples of Underlying Tray Hydraulic Correlations

Aspen Technology used correlations from various sources. Figures 2-6 show how the selected models (red) fit the published correlation curves (black). For more information on the equations used, please refer to the Aspen Plus or Aspen HYSYS in-product documentation (F1 help).

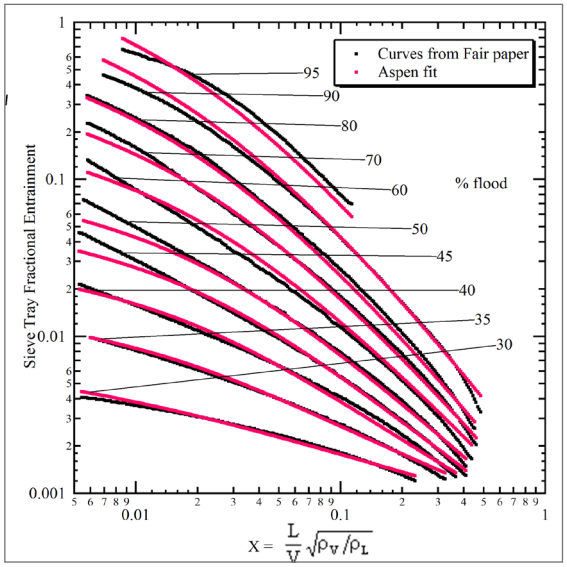

Figure 2: Fractional liquid entrainment correlation for sieve trays[5]

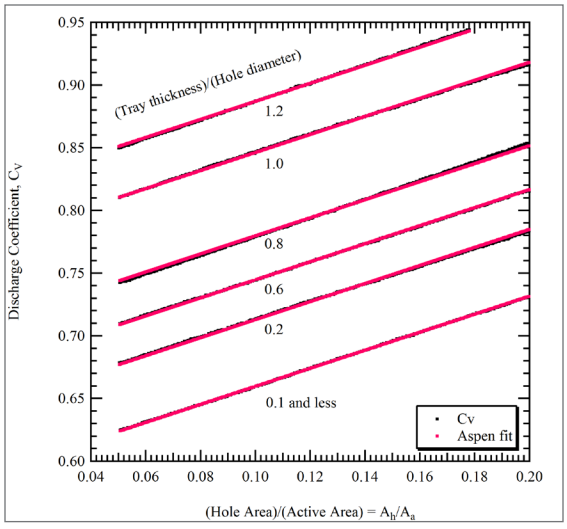

Figure 3: Sieve tray discharge coefficient for vapor flow[5]

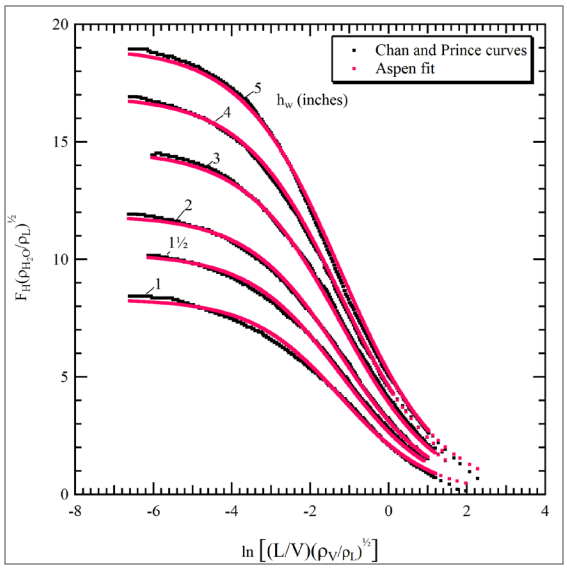

Figure 4: Chan and Prince dump correlation for sieve trays[5]

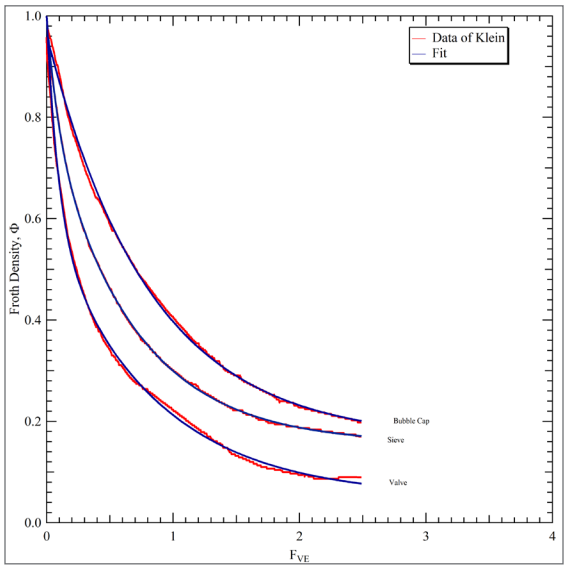

Figure 5: Relative froth density correlations for bubble cap trays, sieve trays and valve trays[8]

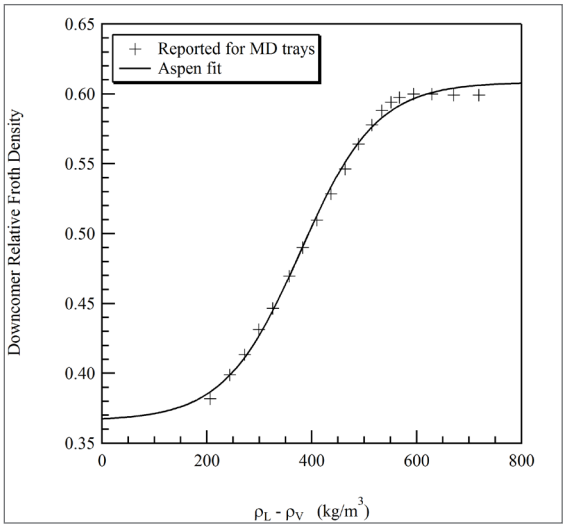

Figure 6: Downcomer relative froth density correlation[7]

Sieve Trays

Better tray hydraulics within Aspen Plus and Aspen HYSYS match KG-TOWER predictions more closely. The following charts show how the model results from Aspen Plus and Aspen HYSYS match KG-TOWER with parity plots, Figures 7-9, and comparison of model results for pressure drop per height to KG-TOWER and experimental data, Figures 10-11. The comparisons were conducted assuming 100% stage efficiency and models were built using the Peng-Robinson equation of state. For these comparisons, temperature and composition profiles were not considered.

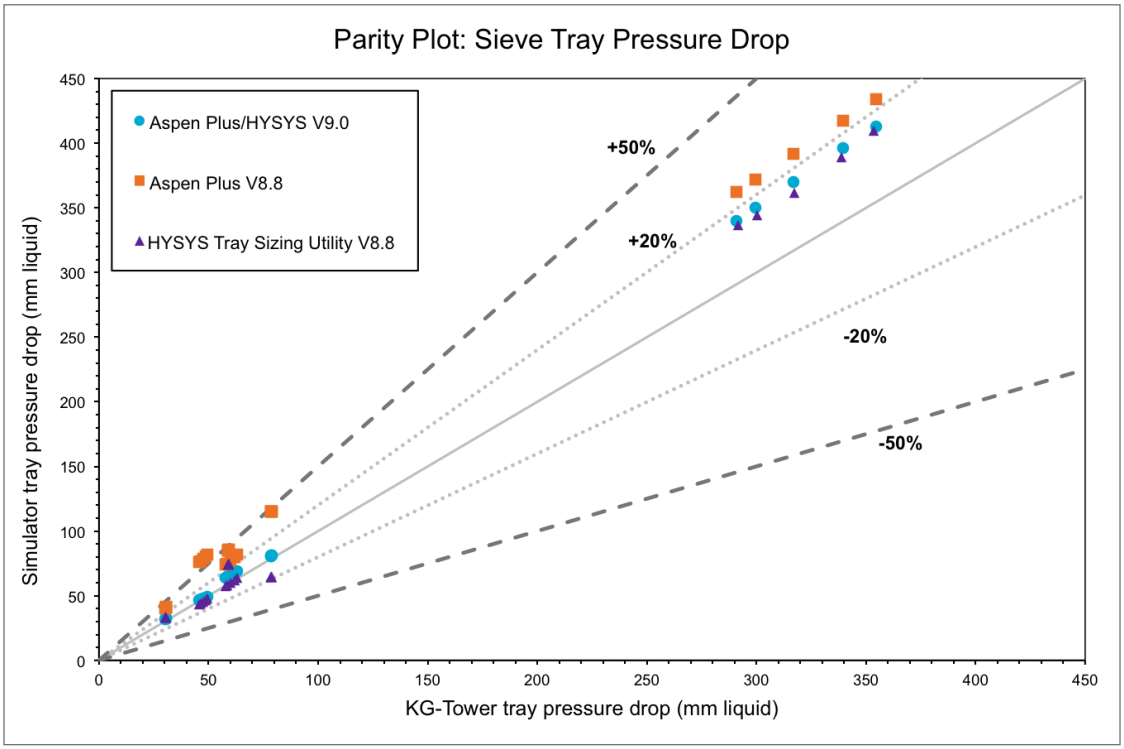

Figure 7: Parity plot comparing sieve tray pressure drops calculated by previous versions of Aspen Plus and Aspen HYSYS and the new versions of Aspen Plus and Aspen HYSYS with those from KG-TOWER.

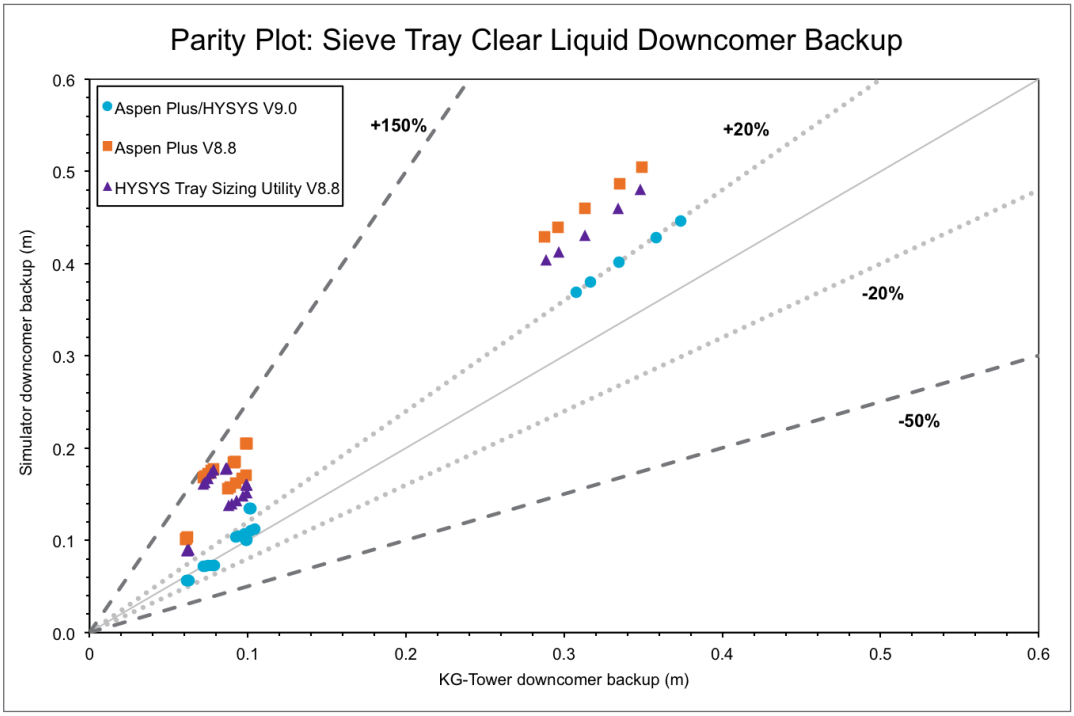

Figure 8: Parity plot comparing sieve tray downcomer backups calculated by previous versions of Aspen Plus and Aspen HYSYS and the new versions of Aspen Plus and Aspen HYSYS with those from KG-TOWER

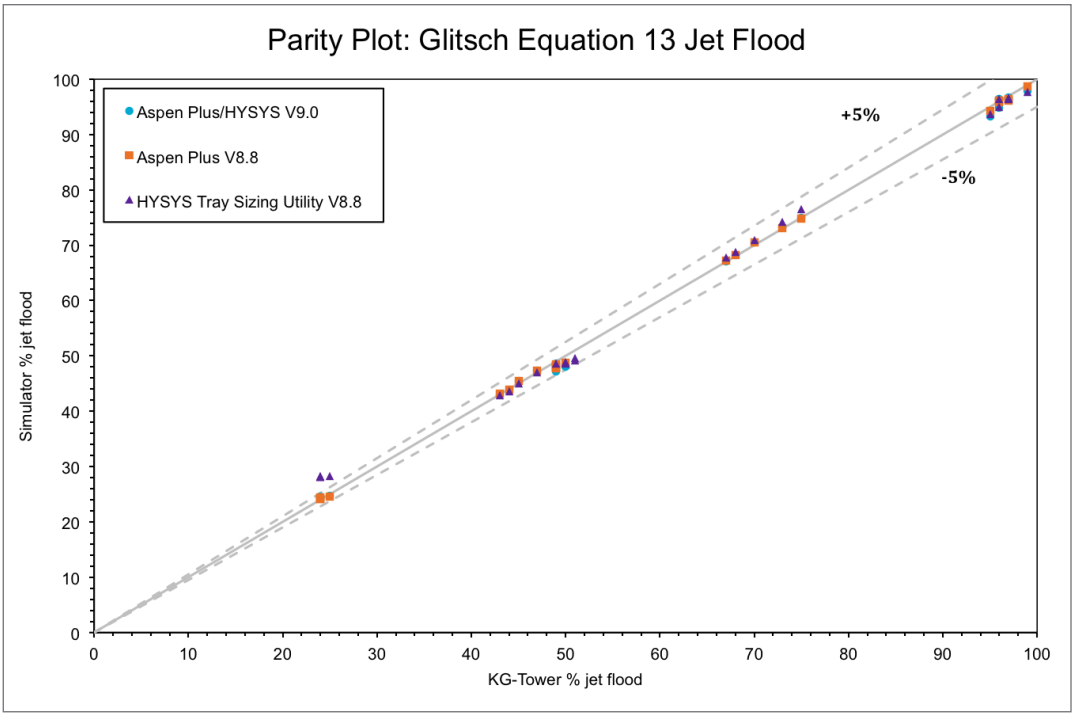

Figure 9: Parity plot comparing sieve tray approaches to jet flood calculated by previous versions of Aspen Plus and Aspen HYSYS and the new versions of Aspen Plus and Aspen HYSYS with those from KG-TOWER. Glistch Equation 13 was used for this comparison.

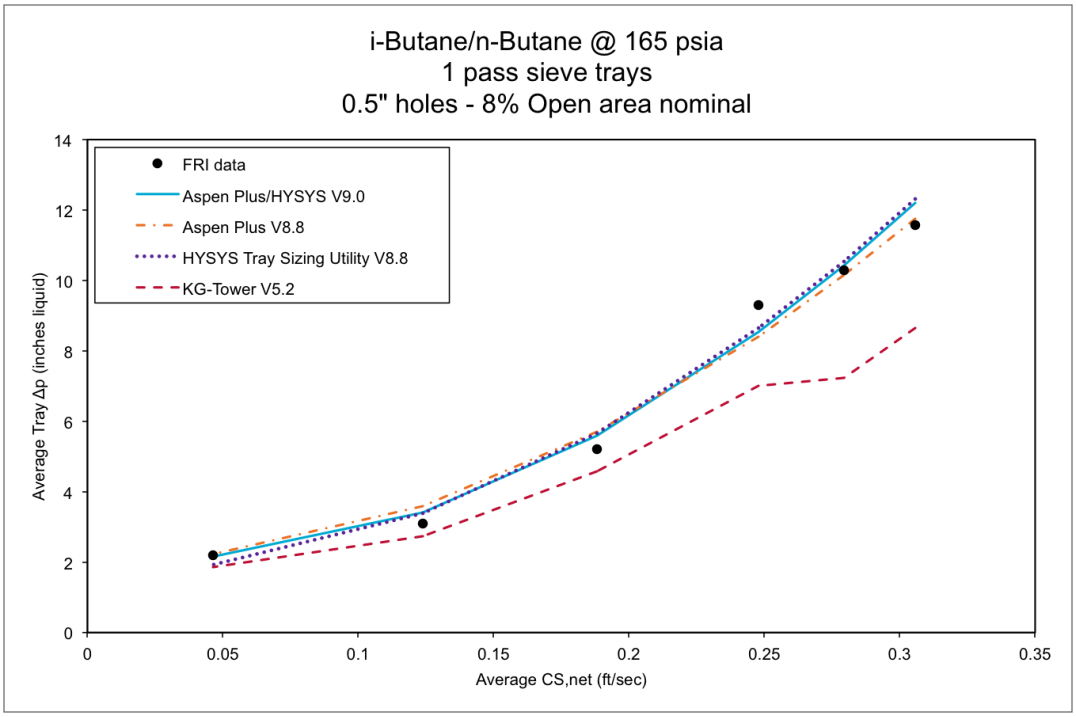

Figure 10: This chart compares the tray pressure drops calculated by the new Column Analysis feature in Aspen Plus and Aspen HYSYS with data from an FRI experiment.[16]

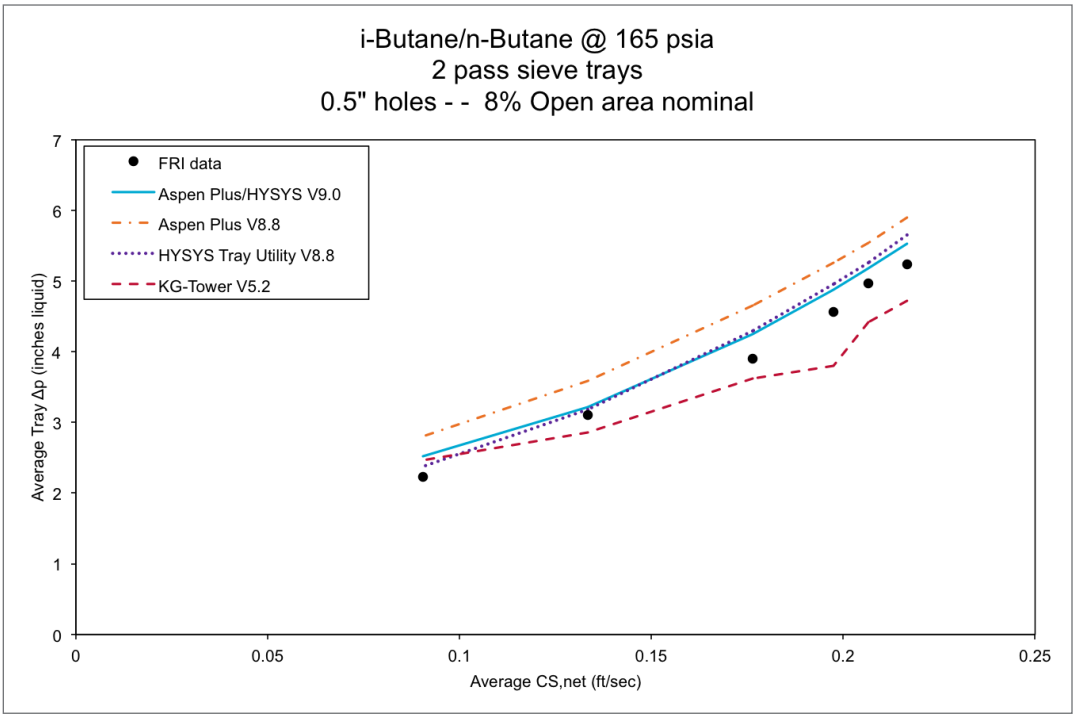

Figure 11: This chart compares the tray pressure drops calculated by the new Column Analysis feature in Aspen Plus and Aspen HYSYS with data from an FRI experiment.[17]

Round Valve Trays

The new Column Analysis feature includes selections for V-1 and V-4 Glistch-Ballast round valve trays which are similar to the R-1 and R-4 valve trays available in Sulzer ChemTech's Sulcol software. Comparisons were conducted between the new Column Analysis features, previous versions of Aspen HYSYS and Aspen Plus, and KG-TOWER and Sulcol software. The trays in the experiment were constructed with swept-back weirs which are not available in previous versions of Aspen Plus and Aspen HYSYS. Because of this additional functionality, Aspen Plus and Aspen HYSYS are better able to predict average tray pressure drops for trays with swept-back weirs. The following charts show how the simulation results match experimental data for pressure drop predictions, Figures 12 and 13. The comparisons were conducted assuming 100% stage efficiency and models were built using the Peng-Robinson equation of state. For these comparisons, temperature and composition profiles were not considered.

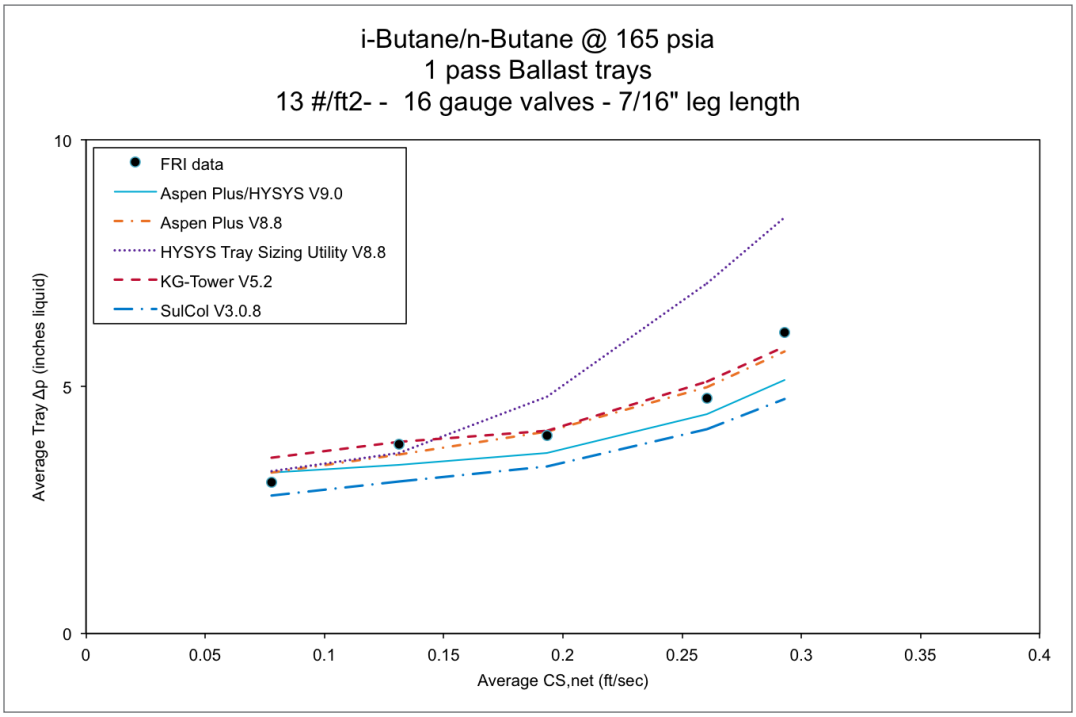

Figure 12: This chart compares the tray pressure drops calculated by the new Column Analysis feature in Aspen Plus and Aspen HYSYS with data from an FRI experiment.[4]

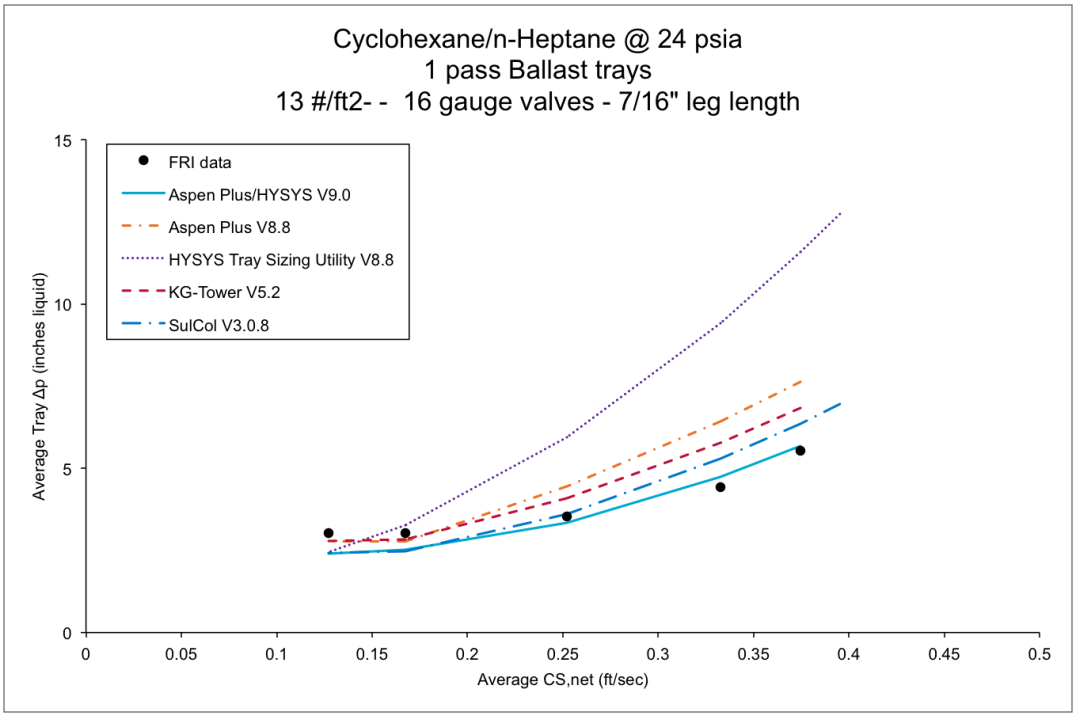

Figure 13: This chart compares the new Column Analysis feature in Aspen Plus and Aspen HYSYS with data from an FRI experiment.[4]

Improvements to Packing Hydraulic Correlations

In addition to improved correlations for tray hydraulics, existing packing hydraulic correlations in Aspen Plus and Aspen HYSYS have been validated with experimental data for multiple packing types. The Aspen-Wallis pressure drop/flood correlation for packings matches data quantitatively and reduces the need for "system factors" in the estimation of column flood points or maximum operating capacities. In almost all cases, the Aspen-Wallis pressure drop correlation better predicts both the pressure drop and the capacity of the system at the flood point than previously used pressure drop correlations. In Aspen HYSYS and Aspen Plus, Aspen-Wallis is the new default correlation used for packing pressure drop correlations (other options are available). Compared to alternative software tools and popular literature correlations, the Aspen-Wallis correlation provides results for packing that are equivalent or more accurate when compared to experimental data. For the following comparisons, an assumption of 100% stage efficiency was used and the Peng-Robinson equation of state was applied when building the models. For these comparisons, temperature and composition profiles were not considered.

Case Study: Revamp of Ethylbenzene/Styrene Splitter

To showcase the accuracy of the Column Analysis results using the Aspen-Wallis pressure drop correlation, a case study of a revamp of an ethylbenzene/styrene splitter with Sulzer's Mellapak™ Plus packing was used. The diagram in Figure 14 shows the column configuration and conditions. Table 1 shows how the reported bottom pressure compares to the four tools.[14]

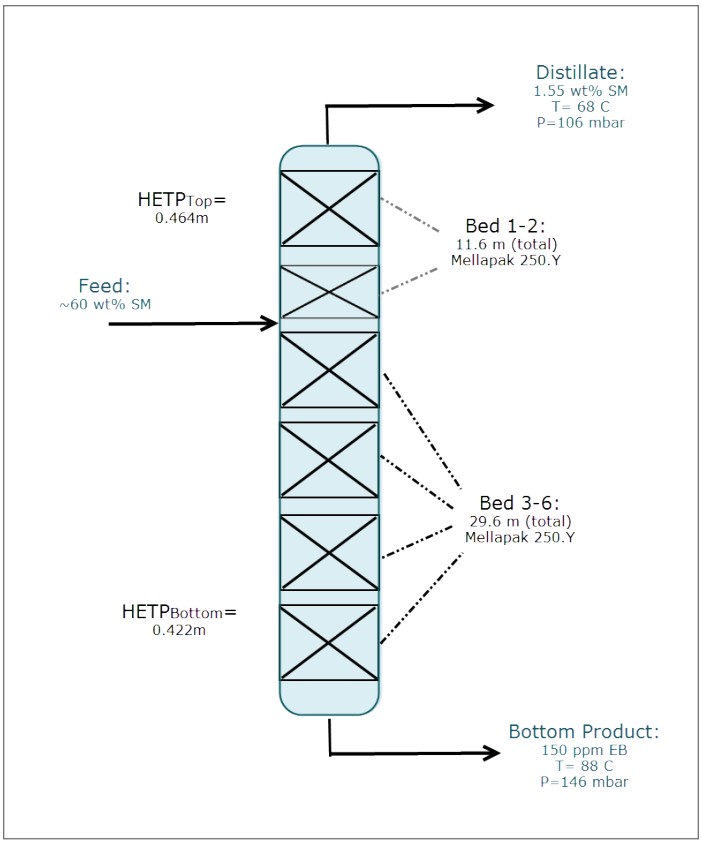

Figure 14: Diagram of the ethylbenzene/styrene splitter example

Correlation	P_{bot} (mbar)	% Flood	% Error
GPDC-85	208.6	67	42.86
Sulcol	149.0	59	2.05
KG-TOWER	152.0	65	4.11
Column Analysis feature in Aspen Plus and Aspen HYSYS*	149.2	65	2.22
Reported Pressure	**146**		

*Using default Aspen-Wallis pressure drop/flood correlation

Table 1: Comparison of the calculation results for the ethylbenzene/styrene splitter example.

Random Packing

Random packings are used when an economical solution is required to increase the capacity of a tower, achieve lower pressure drops and increase separation efficiency. Two types of random packings were studied using the new Aspen-Wallis correlation: Pall Rings and IMTP (and Sulzer equivalents).

Pall Rings

For a Pall Ring comparison, three systems with experimental data were tested. The Aspen-Wallis equation was compared to the SLE correlation, KG-TOWER (v5.2) and Sulcol (V3.0.8).

Methanol/Ethanol

Figures 15 and 16 show comparisons for a 16mm and 25mm Pall ring, respectively, tested for methanol/ethanol separation at 14.7 psia. Data was taken from: Billet R. Recent investigations of metal pall rings. *Chem Eng Prog.* 1967; 63:53.

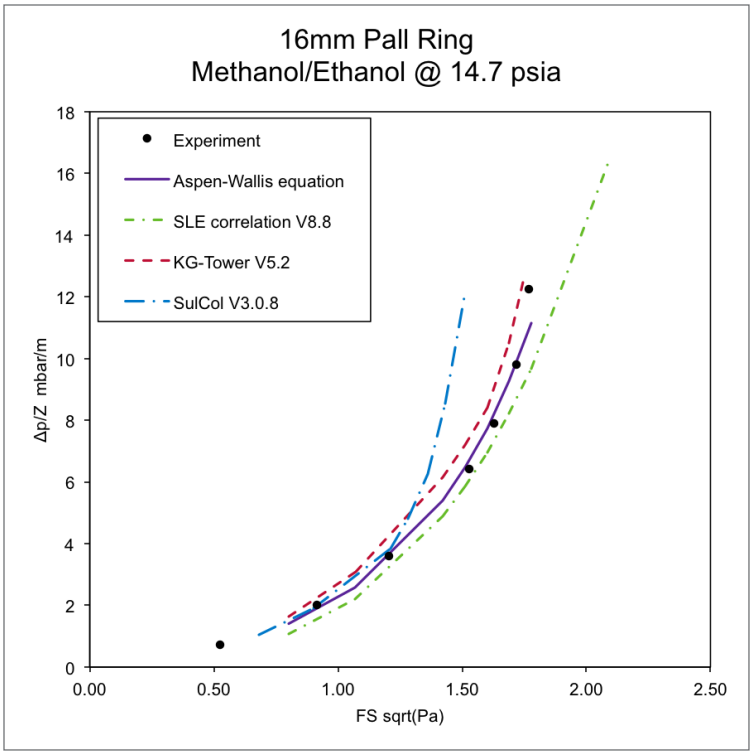

Figure 15: 16mm Pall Rings

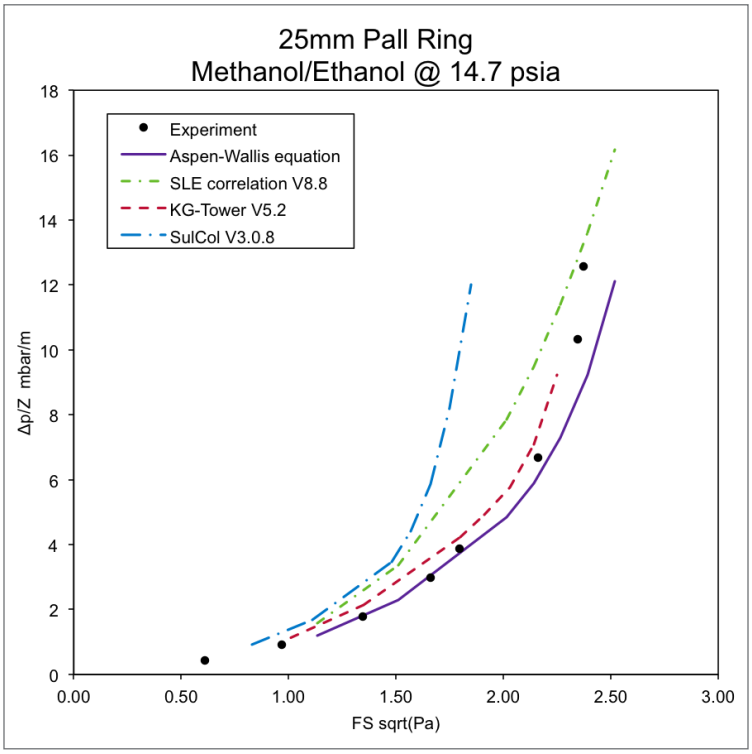

Figure 16: 25mm Pall Rings

Ethylbenzene/Styrene

Figures 17 and 18 show results for 16mm and 25mm Pall rings, respectively, tested for ethylbenzene/styrene separation at 1.93 psia. The Aspen-Wallis equation was compared to SLE correlation in V8.8 of Aspen Plus and Aspen HYSYS, KG-TOWER V5.2 and Sulcol V3.0.8. Data was taken from: Billet R. Recent investigations of metal pall rings. *Chem Eng Prog.* 1967; 63:53.

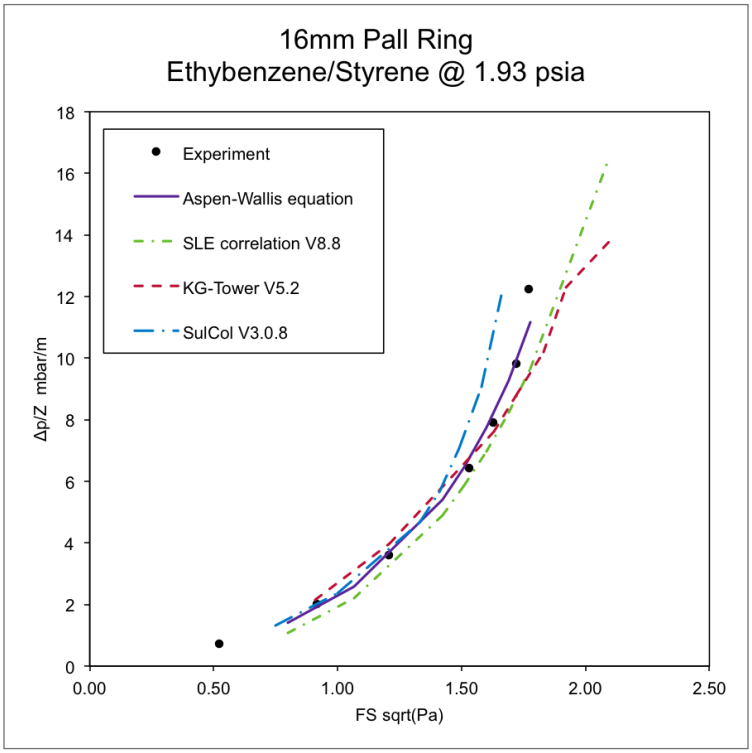

Figure 17: 16mm Pall Rings

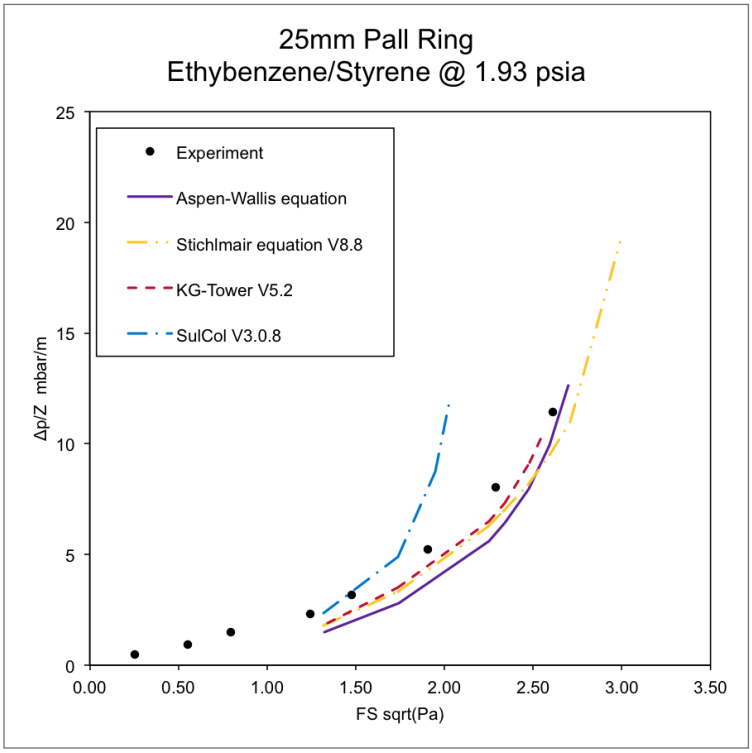

Figure 18: 25mm Pall Rings

Cyclohexane/n-Heptane

Comparison against data for C6/C7 separation was conducted for 50mm Pall Rings at 23.9 psia and is shown in Figure 19. The Aspen-Wallis equation was compared to the Eckert (GPDC) correlation which was the V8.8 default for Aspen Plus, KG-TOWER V5.2 and Sulcol V3.0.8. Experimental Data was taken from: Schultes, M.; Researching rings, *Hydrocarbon Engineering,* Nov. 2001, pp. 57-62.

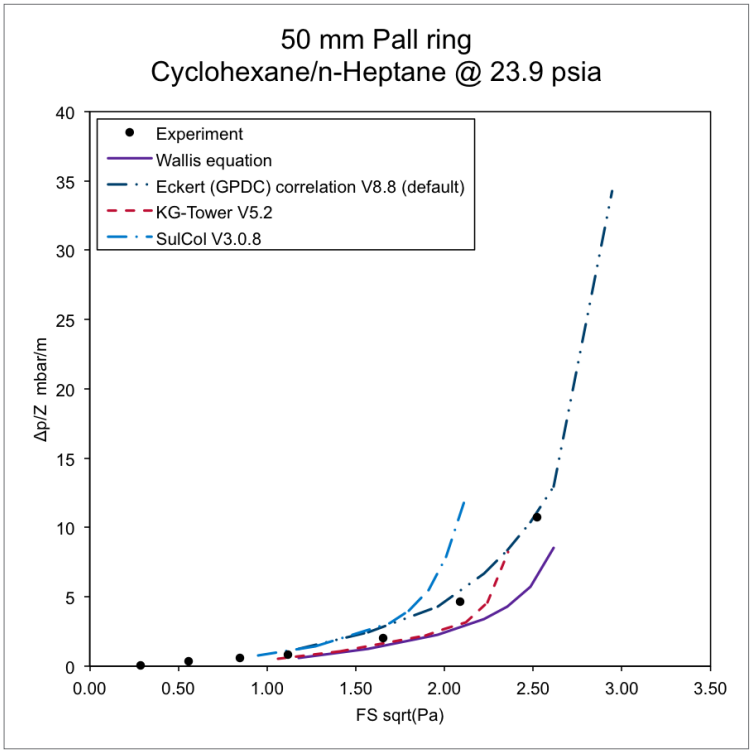

Figure 19: 50mm Pall Ring

IMTP

IMTP random packing was chosen as a second random packing for validation. This is structurally the same as the i-Ring packing from Sulzer ChemTech. The system tested was i-Octane/Toluene separation at 14.3 psia. The Aspen-Wallis correlation was compared against the Norton correlation, KG-TOWER V5.2 and Sulcol V3.0.8. Figures 20 and 21 show the comparisons. (Koshy TD, Rukovena F. Available at: **http://www.cheresources.com**.)

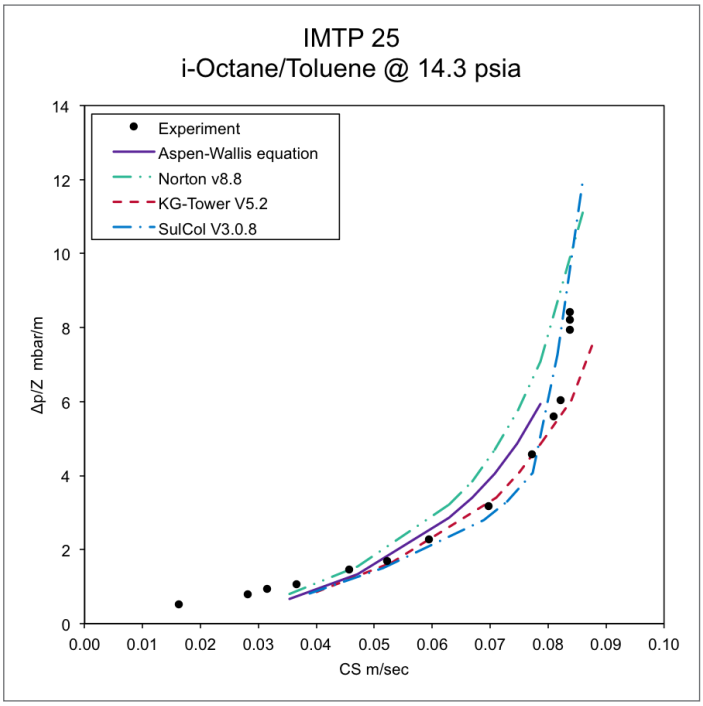

Figure 20: IMTP 25

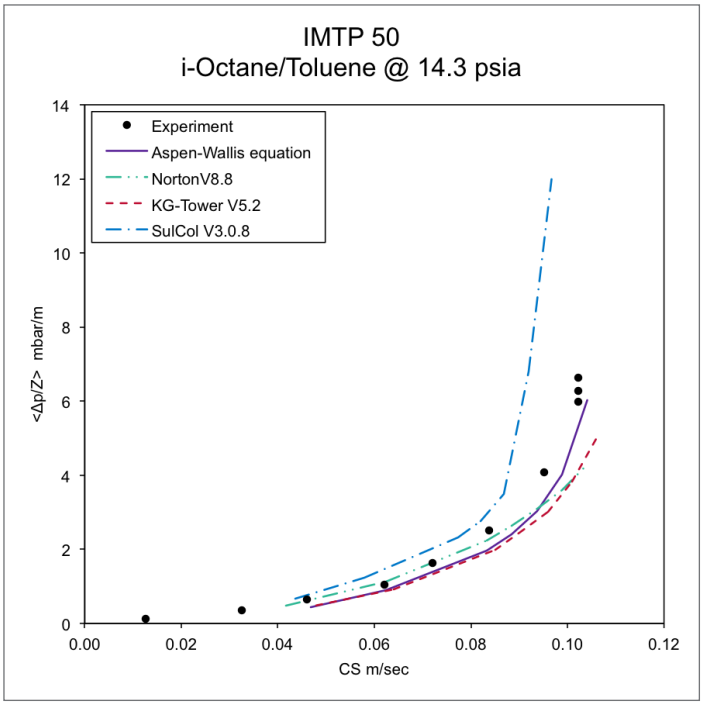

Figure 21: IMTP 50

Structured Packing

Structured packings are used when an even higher capacity, higher separation efficiency and lower pressure drop is needed per theoretical stage. Two structured packings were studied in this analysis: ISP and Mellapak (Sulzer)/ Flexipac (Koch-Glistch).

ISP

The Aspen-Wallis equation was compared against the Norton correlation and KG-TOWER V5.2 and experimental data for i-Octane/Toluene separation at 1.93 psia. The results are shown in Figures 22 and 23. (Koshy TD, Rukovena F. Available at: **http://www.cheresources.com**.)

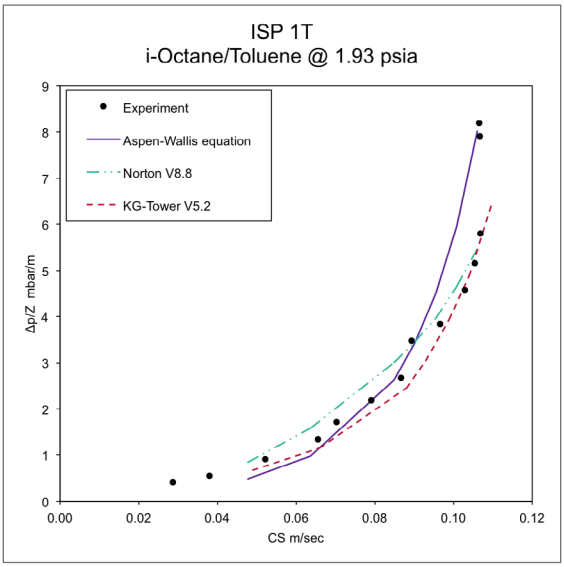

Figure 22: ISP 1T

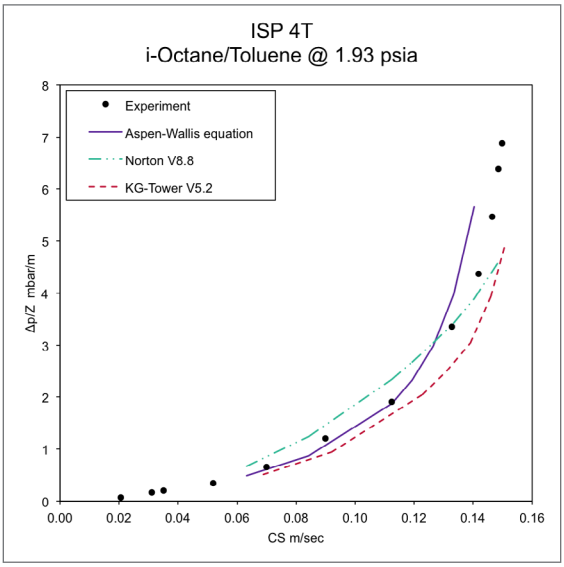

Figure 23: ISP 4T

Mellapak/Flexipac

The Aspen-Wallis equation was compared against the GPDC85 correlation, KG-TOWER V5.2, Sulcol V3.0.8 and experimental data for i-Octane/Toluene separation at 100 psia. As shown in Figure 24, Aspen-Wallis notably matches the experimental data quite well for pressure drop and flood point, simultaneously better than all of the compared correlations.[1]

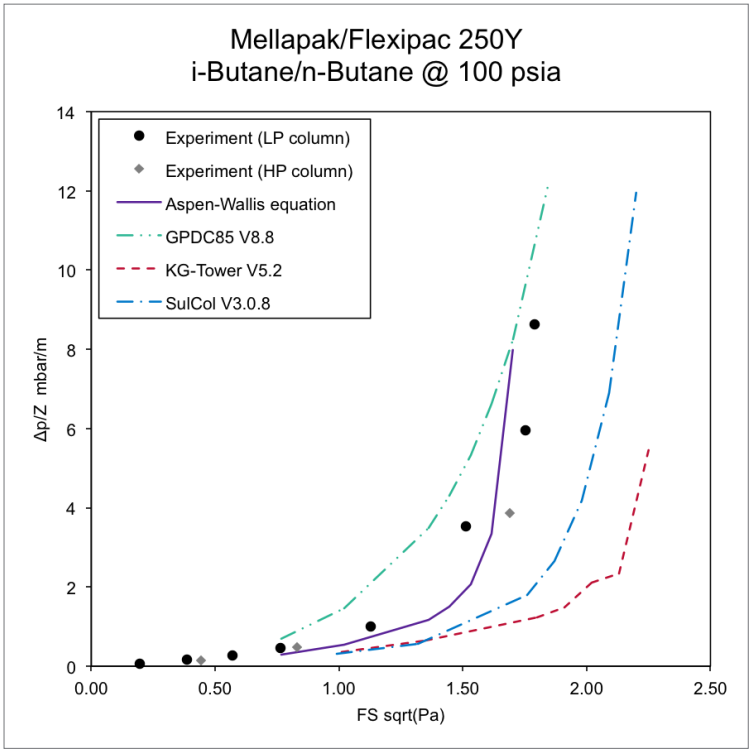

Figure 24: Mellapak/Flexipac 250Y

Conclusion

The new Column Analysis feature within Aspen Plus and Aspen HYSYS gives the user the ability to send geometry and hydraulic information for selected trays to tray/packing rating programs, KG-TOWER and Sulcol, which are readily available.

In Aspen Plus and Aspen HYSYS V9, the results from upgraded correlations show closer agreement with plant data and results from vendor software packages. For packed internals especially, the Aspen-Wallis default pressure drop correlation has been shown to match pressure drop and pressure drop at flood and capacity simultaneously better than other published correlations when compared to plant data. This helps to minimize the need for "system factors" and "safety factors", which in turn means less uncertainty in simulation results.

List of Important Symbols

A_a	"Active" or "bubbling" area of the tray
A_h	Cumulative area of holes on the sieve tray deck
C_d	Liquid gradient factor
C_L	Density corrected superficial liquid velocity. Often, the density correction is taken to be unity.
C_S	Density corrected superficial vapor velocity. For trays, the net area is typically used in the velocity definition ($C_{S,net}$). For packed columns, the cross-sectional area of the column is used.
C_V	Vapor load correction factor for liquid gradient
F_H	Hole F-factor $u_H\sqrt{\rho_V}$
g	Gravitational acceleration
GPM	Liquid rate in gallons per minute
h_{lo}	Height of clear liquid at overflow weir (inches)
L	Liquid mass rate
V	Vapor mass rate
X	Flow parameter $\left(\frac{L}{V}\right)\sqrt{\rho_V/\rho_L}$
ρ_{H2O}	Mass density of water
ρ_L	Liquid mass density
ρ_V	Vapor mass density
Δ	Liquid gradient for tray (inches)
Δ'	$= C_V \Delta$
$\Delta p/Z$	Pressure drop per unit height

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