What's New in *ChemSep*™ 7.4

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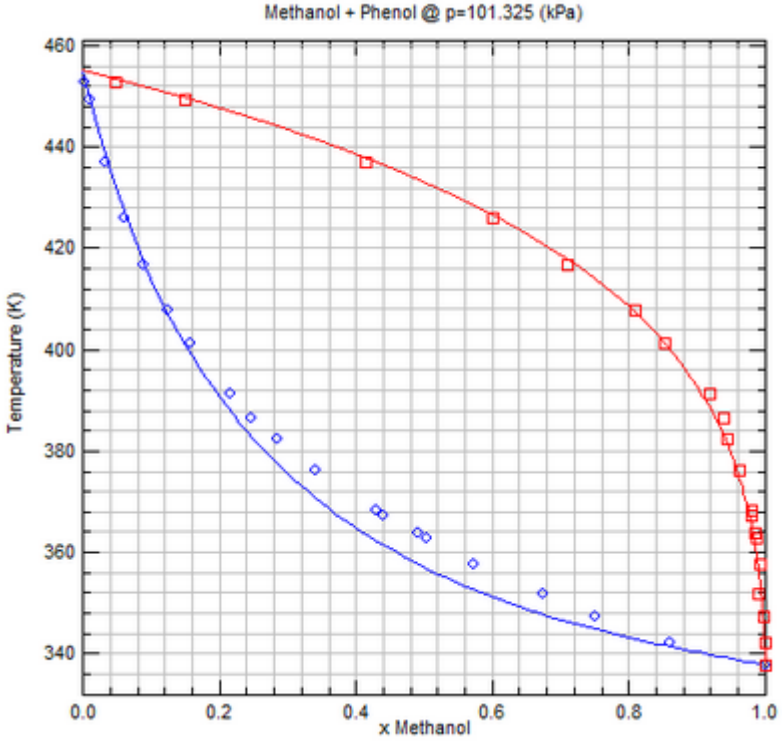
Harry Kooijman and Ross Taylor

UNIFAC (NIST)

We added the UNIFAC group contribution method by NIST Thermodynamics Research Center (TRC) and access to the Viginia Tech (VT) COSMO databank. The UNIFAC (NIST) was defined with more main groups (89) and fitted on VLE, LLE, and SLE data with more group interaction parameters (984) than the original UNIFAC (FPE388p128) and will provide much better descriptions of vapor-liquid equilibria in distillation column simulations than the original UNIFAC. The VT sigma profiles will be used in COSMO-based activity and equation of state thermodynamic models. Here is a Txy diagram for the Methanol-Phenol system for which the standard UNIFAC performs rather poor.



Direct Export of Columns to COCO Flowsheet

Under the file menu you find an “Export to flowsheet” option that allows you to directly export your simulation as flash or column operation in the COCO simulator. The ChemSep properties are simultaneously exported as ChemSep Cape-Open Property Package (CS/COPP) such that the simulation is guaranteed to give the same anwsers as in the stand-alone simulation.

Miscellaneous Updates

Version 7.4 includes many small improvements such as:

- Improved handling of fitting of group interaction parameters
- Allowing guesses for fractional recovery
- Allowing users to extend existing group contribution methods with own groups and to fit the group-group interaction parameters
- writing of compressed SulColZ files (in the rating panel)
- bug fix in the automated assignment of key compounds for the McCabe-Thiele diagrams

Availability

As always, *ChemSep* Lite is available free from http://chemsep.com.