

What's New in ChemSep™ 6.6

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In this document we identify and describe the most important new features in *ChemSep*.

1. **Back Again: Temperature-dependent interaction parameters for VLE**
2. **Improved: Temperature-dependent properties in the databank manager**
3. **New: Excel export from the physical properties databank management program**
4. **New: Easy comparisons of total reflux measurements with simulation results**
5. **New: GUI can directly load ChemSep columns from COCO flowsheet files**

Back again: Temperature dependent interaction parameters

Temperature-dependent parameters for activity coefficient models can be employed in ChemSep again.

This option is available for the Wilson, NRTL, and UNIQUAC activity coefficient models. The default choice is *None* (meaning the parameters are independent of temperature). To select a particular temperature dependent format click on the expression list that appears in the top-right corner of the illustration below.

Enter Thermodynamic Model Parameters (when required)

UNIQUAC UNIQUAC Units K T dependence A + D.T + F.T.T

Reset Load Save

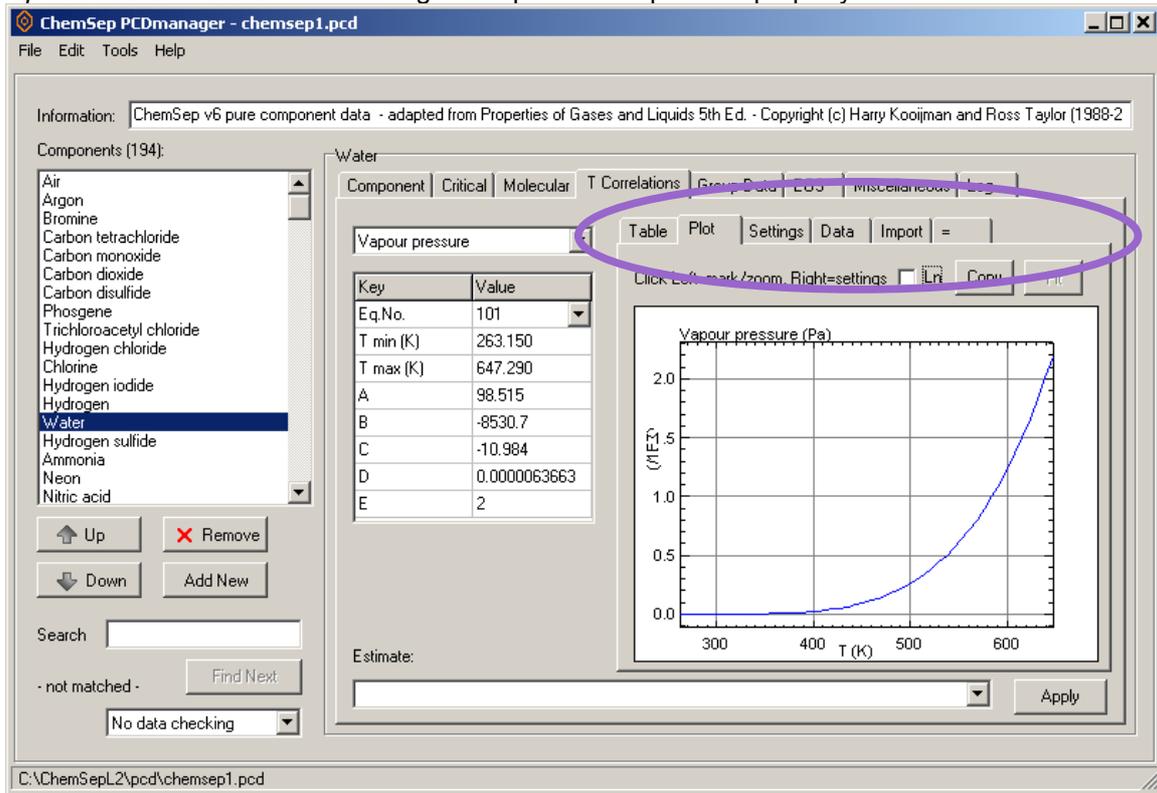
i - j	A-ij	A-ij	D-ij	D-ij	
Acetic acid - Methanol	390.260	65.2450	0.970390	-2.03460	
Acetic acid - Methyl acetal	-62.1860	81.8480	-0.436370	1.11620	
Acetic acid - Water	422.380	-98.1200	-0.0510070	-0.29355	
Methanol - Methyl acetate	62.9720	326.200	-0.710110	0.724760	0.00116700
Methanol - Water	-575.680	219.040	3.14530	-2.05850	-6.071E-03
Methyl acetate - Water	593.700	-265.830	0.0101430	0.962950	-2.160E-03

None
A + B/T
A + B/T + C.ln(T)
A + D.T
A + D.T + F.T.T
A + B/T + D.T

Important note: The *Units* in the above represents the units of the parameter calculated from these expressions; it does not refer to the units of the individual constants such as *A*, *B*, etc.

Improved: Properties Data Manager

ChemSep 6.6 features enhanced handling of temperature dependent property correlations.



Note the new set of tabs contained within the ellipse in the above screen shot. For more information see www.chemsep.com/downloads/docs/ChemSepTutorial_PCDManager.pdf

New: Extracting Physical Property Constants to Excel

In Version 6.5 we introduced a new and vastly improved capability of exporting simulation input and results to Excel. In version 6.6 we have brought that capability to the physical properties databank management program we call PCDmanager. The illustration below shows a table in Excel created using this new capability.

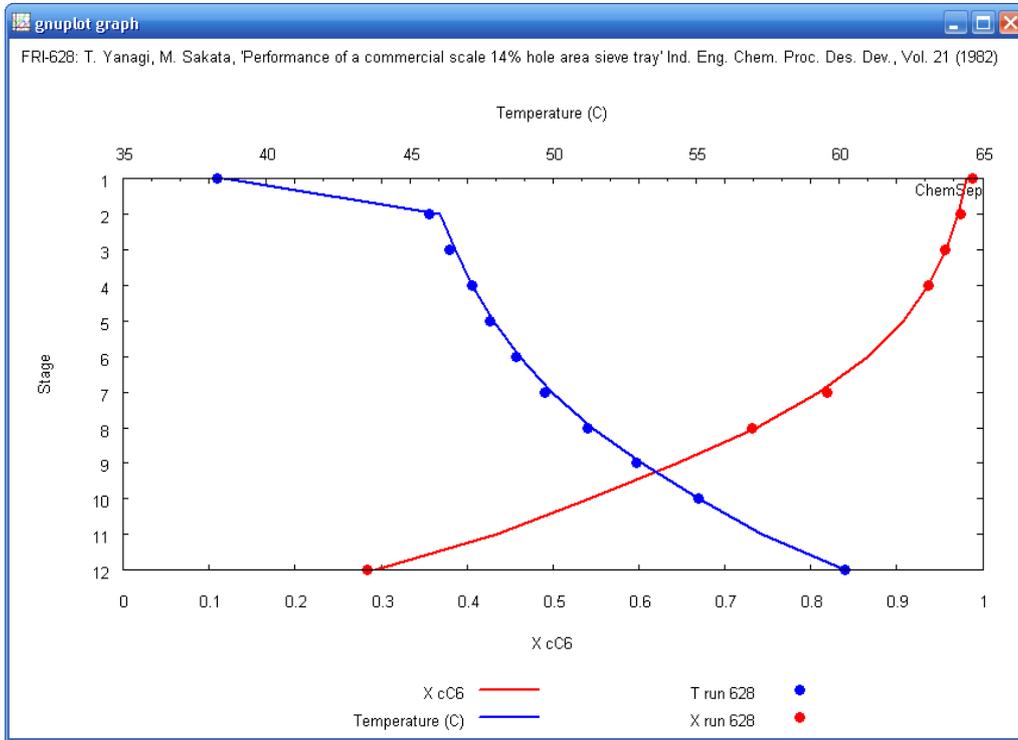
The screenshot shows a Microsoft Excel spreadsheet with the following data:

Name	Formula	Mw	SG	Tboil	Tmelt
		kg/kmol		C	F
Air		28.96		-194.48	-353.2
Argon	Ar	39.948	1.37018	-185.88	-308.823
Bromine	Br2	159.808		58.75	18.94999
Carbon tetrachloride	CCl4	153.822	1.60128	76.64001	-9.076
Carbon monoxide	CO	28.01	0.799388	-191.49	-337
Carbon dioxide	CO2	44.0095			-69.826
Carbon disulfide	CS2	76.1407	1.26931	46.22501	-168.826
Phosgene	CCl2O	98.9161	1.381	7.559998	-198.004
Trichloroacetylene	C2Cl4O	181.833	1.62992	118	-70.51
Hydrogen chloride	HCl	36.461	0.854783	-85	-173.524
Chlorine	Cl2	70.905	1.41956	-34.03	-149.854
Hydrogen iodide	HI	127.912	2.54382	-35.6	-59.386
Hydrogen	H2	2.01588	0.069859	-252.76	-434.56
Water	H2O	18.015	0.997986	100	31.99999
Hydrogen sulfide	H2S	34.0809		-60.35	-121.846
Ammonia	H3N	17.031	0.618067	-33.33	-107.932

For more information please see the tutorial at www.chemsep.com/downloads/docs/ChemSepTutorial_PCExport.pdf

New: Easy Comparisons of Total Reflux Data with Simulation Results

In the MS Windows version of ChemSep we introduced total reflux simulations and showed how to make comparisons of measured temperature and liquid composition profiles in Microsoft Excel. Such plots can now be more easily made inside ChemSep, as illustrated below. The distribution comes with example files (fri*.sep).



New: Load ChemSep Columns Residing in COCO Flowsheet Files

In Version 6.6 we allow direct loading of any ChemSep column from COCO flowsheet files! If multiple columns reside in the FSD files a list of column names is shown for the user to select. The columns are loaded in stand-alone mode i.e. they are saved as sep-files residing outside the flowsheet. This allows the user not only to inspect results but also to solve these columns - but then using ChemSep internal property routines.