DWSIM 3

Excel Add-In User Guide

Introduction

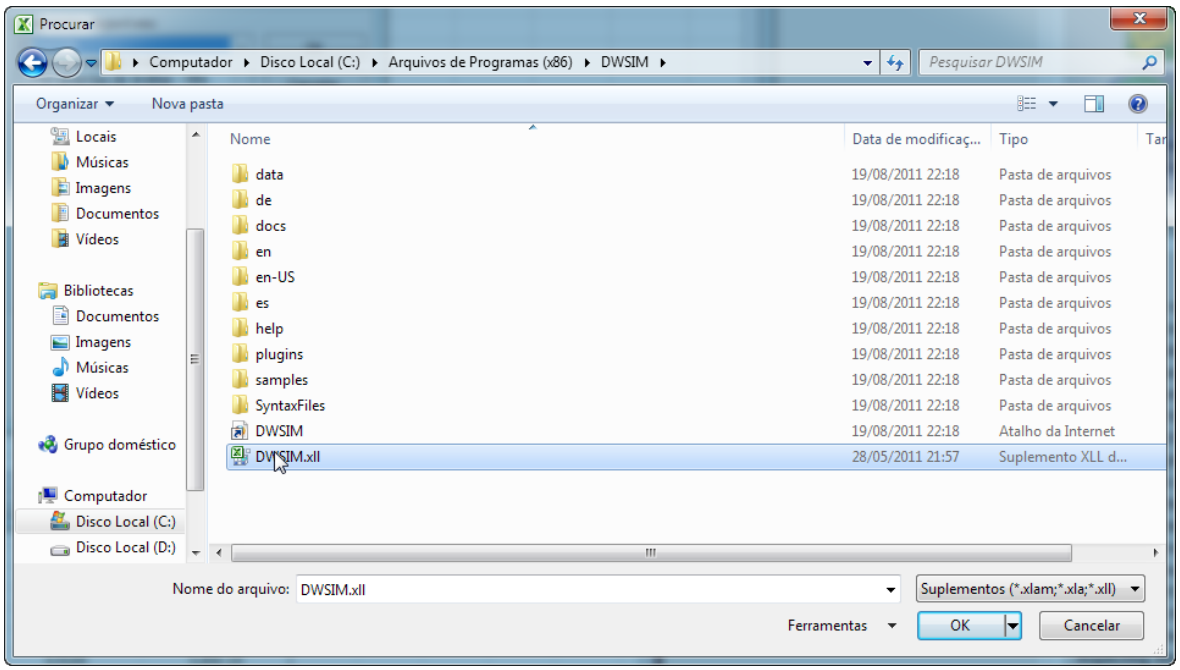
The DWSIM Excel Add-In enables usage of some low-level internal functions in DWSIM, exposed so far only to CAPE-OPEN compatible software. Some of the functions exposed include:

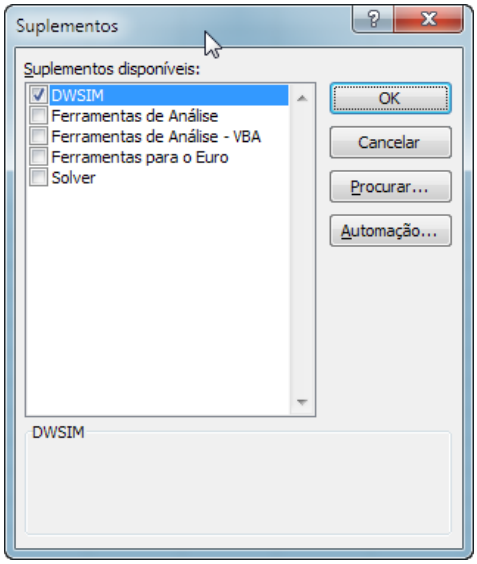
- Single Compound Property Calculator
- Single Phase Mixture Property Calculator
- PT, PH, PS, PVF and TVF Flash Calculators, using an algorithm of your choice
- Other auxiliary functions

Property and Equilibrium calculation functionality is now available to Excel just as any other add-in function.

Installation

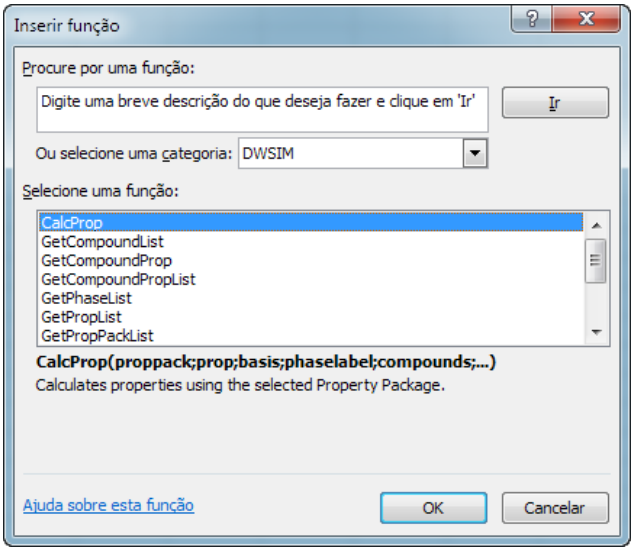
The Excel add-in can be installed using the normal procedure for XLL add-ins. Just look for the “DWSIM.xll” file in the DWSIM installation directory and you’re set:



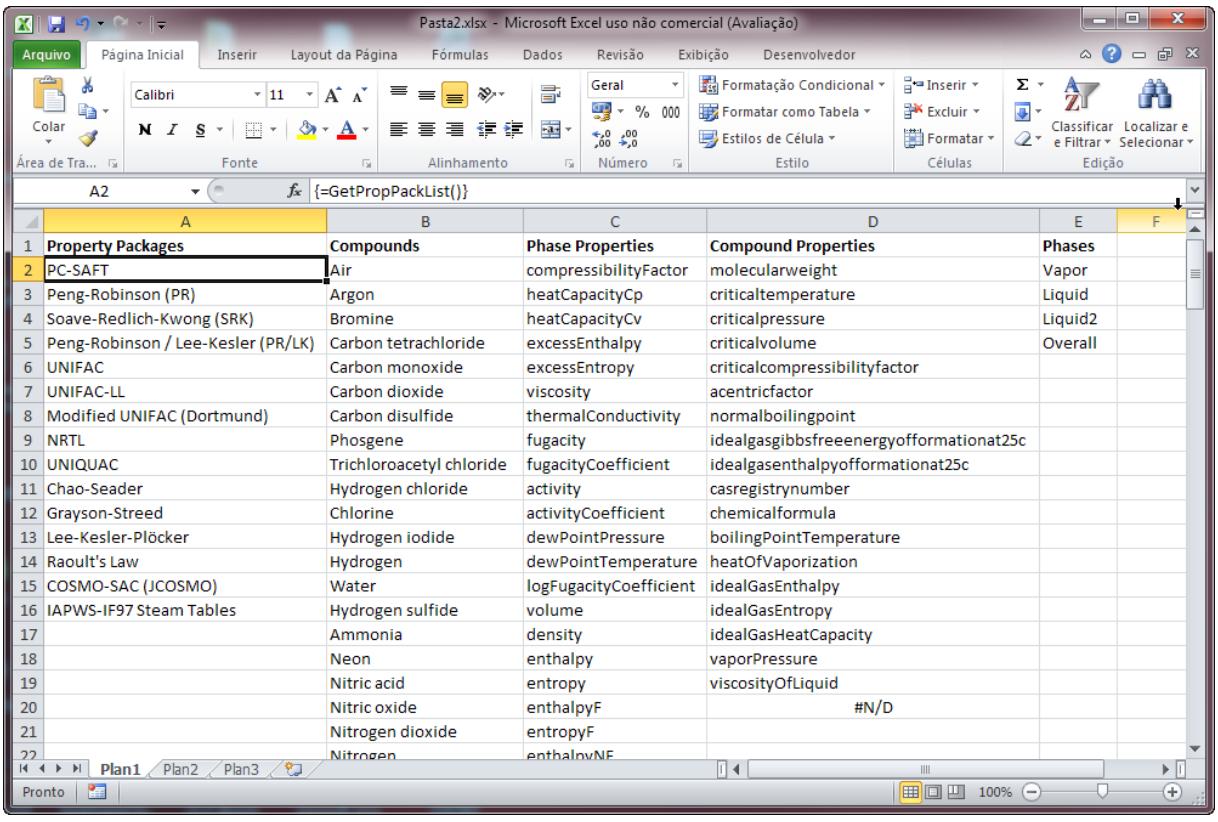


Usage

Functions exposed by this add-in will be grouped in a category named “DWSIM”:

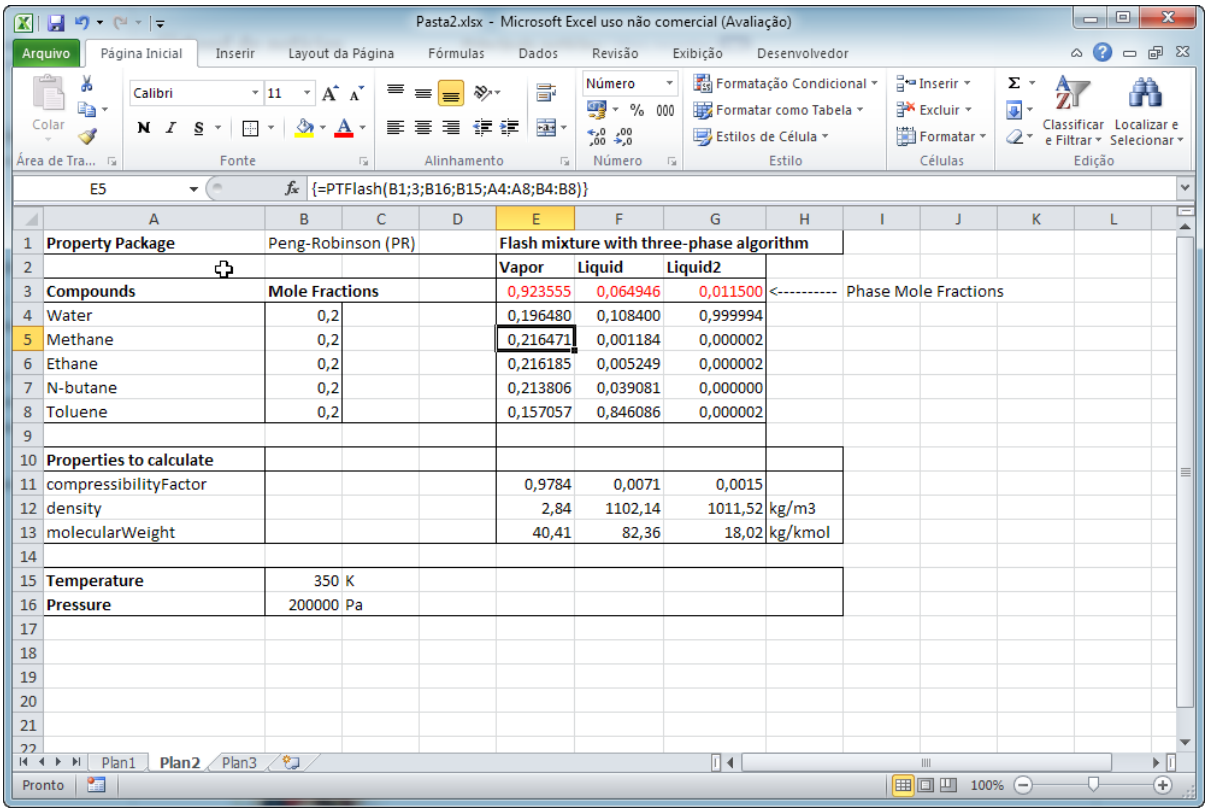


Property and Equilibrium calculation functions require parameters that must be one or more values returned by ***GetPropPackList***, ***GetCompoundList***, ***GetPropList***, ***GetCompoundPropList*** and ***GetPhaseList***. They are self-explanatory, and will return values listed in a single column, so you probably will have to select some cells in a single column and call the functions using *Ctrl+Shift+Enter*:



	A	B	C	D	E	F
1	**Property Packages**	**Compounds**	**Phase Properties**	**Compound Properties**	**Phases**	
2	PC-SAFT	Air	compressibilityFactor	molecularweight	Vapor	
3	Peng-Robinson (PR)	Argon	heatCapacityCp	criticaltemperature	Liquid	
4	Soave-Redlich-Kwong (SRK)	Bromine	heatCapacityCv	criticalpressure	Liquid2	
5	Peng-Robinson / Lee-Kesler (PR/LK)	Carbon tetrachloride	excessEnthalpy	criticalvolume	Overall	
6	UNIFAC	Carbon monoxide	excessEntropy	criticalcompressibilityfactor		
7	UNIFAC-LL	Carbon dioxide	viscosity	acentricfactor		
8	Modified UNIFAC (Dortmund)	Carbon disulfide	thermalConductivity	normalboilingpoint		
9	NRTL	Phosgene	fugacity	idealgasgibbsfreeenergyofformationat25c		
10	UNIQUAC	Trichloroacetyl chloride	fugacityCoefficient	idealgasenthalpyofformationat25c		
11	Chao-Seader	Hydrogen chloride	activity	casregistrynumber		
12	Grayson-Streed	Chlorine	activityCoefficient	chemicalformula		
13	Lee-Kesler-Plöcker	Hydrogen iodide	dewPointPressure	boilingPointTemperature		
14	Raoult's Law	Hydrogen	dewPointTemperature	heatOfVaporization		
15	COSMO-SAC (JCOSMO)	Water	logFugacityCoefficient	idealGasEnthalpy		
16	IAPWS-IF97 Steam Tables	Hydrogen sulfide	volume	idealGasEntropy		
17		Ammonia	density	idealGasHeatCapacity		
18		Neon	enthalpy	vaporPressure		
19		Nitric acid	entropy	viscosityOfLiquid		
20		Nitric oxide	enthalpyF	#N/D		
21		Nitrogen dioxide	entropyF			
22		Nitrogen	enthalpyNF			

For example, the ***PTFlash*** function requires the name of the Property Package to use, the compound names and mole fractions, temperature in K, pressure in Pa and you may optionally provide new interaction parameters that will override the ones used internally by DWSIM. The calculation results will be returned as a *(n+2) x (3)* matrix, where *n* is the number of compounds. First row will contain the phase names, the second will contain the phase mole fractions and the other lines will contain the compound mole fractions in the corresponding phases:



	A	B	C	D	E	F	G	H	I	J	K	L
1	**Property Package**	Peng-Robinson (PR)			**Flash mixture with three-phase algorithm**							
2					**Vapor**	**Liquid**	**Liquid2**					
3	**Compounds**	**Mole Fractions**			0,923555	0,064946	0,011500	<----------	Phase Mole Fractions			
4	Water	0,2			0,196480	0,108400	0,999994					
5	Methane	0,2			0,216471	0,001184	0,000002					
6	Ethane	0,2			0,216185	0,005249	0,000002					
7	N-butane	0,2			0,213806	0,039081	0,000000					
8	Toluene	0,2			0,157057	0,846086	0,000002					
9												
10	**Properties to calculate**											
11	compressibilityFactor				0,9784	0,0071	0,0015					
12	density				2,84	1102,14	1011,52	kg/m3				
13	molecularWeight				40,41	82,36	18,02	kg/kmol				
14												
15	**Temperature**	350	K									
16	**Pressure**	200000	Pa									
17												
18												
19												
20												
21												
22												

For PH, PS, TVF and PVF flash calculation functions, and additional line is returned that will contain the temperature in K or pressure in Pa in the first column.

Overriding Interaction Parameters

You can directly override the interaction parameters used by Property Packages when calling calculations from Excel by providing *n x n* matrices containing the values, where *n* is the number of compounds. **This feature is optional and should be used only when you know exactly what you are doing**.

The following table shows the user-definable interaction parameters for each Property Package:

Property Package	IP Set #1	IP Set #2	IP Set #3	IP Set #4	IP Set #5	IP Set #6	IP Set #7	IP Set #8
PC-SAFT	PC-SAFT kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Peng-Robinson (PR)	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Soave-Redlich-Kwong (SRK)	SRK kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Peng-Robinson-Stryjek-Vera 2 (PRSV2)	PRSV2-M kij	PRSV2-M kji	Not used	Not used	Not used	Not used	Not used	Not used
Peng-Robinson / Lee-Kesler (PR/LK)	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
UNIFAC	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
UNIFAC-LL	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Modified UNIFAC (Dortmund)	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
NRTL	PR kij	NRTL A12 (cal/mol)	NRTL A21 (cal/mol)	NRTL Alpha	NRTL B12 (cal/mol.K)	NRTL B21 (cal/mol.K)	NRTL C12 (cal/mol.K²)	NRTL C21 (cal/mol.K²)
UNIQUAC	PR kij	UNIQUAC A12 (cal/mol)	UNIQUAC A21 (cal/mol)	UNIQUAC B12 (cal/mol.K)	UNIQUAC B21 (cal/mol.K)	UNIQUAC C12 (cal/mol.K²)	UNIQUAC C21 (cal/mol.K²)	Not used
Chao-Seader	Not used	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Grayson-Streed	Not used	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Lee-Kesler-Plöcker	LKP kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
Raoult's Law	Not used	Not used	Not used	Not used	Not used	Not used	Not used	Not used
COSMO-SAC (JCOSMO)	PR kij	Not used	Not used	Not used	Not used	Not used	Not used	Not used
IAPWS-IF97 Steam Tables	Not used	Not used	Not used	Not used	Not used	Not used	Not used	Not used