DWSIM Standalone Thermodynamics Library
User Guide

Introduction

The DWSIM Standalone Thermodynamics Library is a .NET/Mono managed dynamic link library (DLL) that exposes DWSIM's thermodynamics engine to external applications using a simple programming interface, with no dependency on external components.

DWSIM Standalone Thermodynamics Library is free for commercial and non-commercial use. Read the license.txt file for more details.

Usage

To start using the library, add a reference to **DWSIM.Thermodynamics.dll** to your project. All calculation functions will be available in the *DTL.Thermodynamics* namespace, *Calculator* class.

Some of the available functions in this library include:

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

Methods

Property and Equilibrium calculation functions require parameters that must be one or more values returned by ***GetPropPackList***, ***GetCompoundList***, ***GetPropList***, ***GetCompoundConstPropList,*** ***GetCompoundTDepPropList, GetCompoundPDepPropList*** and ***GetPhaseList***. They are self-explanatory, and will return values in an array of strings.

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 the library. The calculation results will be returned as a *(n+2) x (3)* string 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.

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

Property Package Method and Correlation Profiles

The following table lists the methods and correlations used by the Property Packages to do the requested calculations. Experimental data is used whenever available to calculate thermal conductivity and viscosity values.

Details about the thermodynamic methods and correlations used by this library can be found in the technical guide.

	Vapor Phase					Liquid Phases				
	Fugacity	Enthalpy Entropy Cp/Cv	Thermal Conductivity	Viscosity	Density	Fugacity	Enthalpy Entropy Cp/Cv	Thermal Conductivity	Viscosity	Density
Peng-Robinson (PR)	EOS	EOS	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	EOS	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
Peng-Robinson-Stryjek-Vera 2 (PRSV2)	EOS	EOS	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	EOS	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
Soave-Redlich-Kwong (SRK)	EOS	EOS	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	EOS	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
Peng-Robinson / Lee-Kesler (PR/LK)	EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
UNIFAC	PR EOS	LK	Exp./Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	PR EOS	UNIFAC	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
UNIFAC-LL	PR EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	PR EOS	UNIFAC-LL	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
Modified UNIFAC (Dortmund)	PR EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	PR EOS	MODFAC	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
NRTL	PR EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	PR EOS	NRTL	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/Rackett
UNIQUAC	PR EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	PR EOS	UNIQUAC	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/Rackett
Chao-Seader	EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	LK	Exp./ Latini	Exp./ Letsou-Stiel	EOS/ Rackett
Grayson-Streed	EOS	LK	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	LK	Exp./ Latini	Exp./ Letsou-Stiel	Rackett
Lee-Kesler-Plöcker	EOS	EOS	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	EOS	EOS	EOS	Exp./ Latini	Exp./ Letsou-Stiel	Rackett
Raoult's Law	Ideal	Ideal	Exp./ Ely-Hanley	Lucas/ Jossi-Stiel-Thodos	Ideal	Ideal	Ideal	Exp./ Latini	Exp./ Letsou-Stiel	Rackett
IAPWS-IF97 Steam Tables	Tables	Tables	Tables	Tables	Tables	Tables	Tables	Tables	Tables	Tables

Overriding Binary Interaction Parameters

You can override the binary interaction parameters (BIPs) used by Property Packages when calling property and equilibrium calculations by providing *n x n* matrices containing the BIP 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 interaction parameters that can be overridden on each Property Package:

Property Package	IP Set #1	IP Set #2	IP Set #3	IP Set #4
Peng-Robinson (PR)	PR kij	Not used	Not used	Not used
Soave-Redlich-Kwong (SRK)	SRK kij	Not used	Not used	Not used
Peng-Robinson-Stryjek-Vera 2 (PRSV2)	PRSV2 kij	PRSV2 kji	Not used	Not used
Peng-Robinson / Lee-Kesler (PR/LK)	PR kij	Not used	Not used	Not used
UNIFAC	PR kij	Not used	Not used	Not used
UNIFAC-LL	PR kij	Not used	Not used	Not used
Modified UNIFAC (Dortmund)	PR kij	Not used	Not used	Not used
NRTL	PR kij	NRTL A12 (cal/mol)	NRTL A21 (cal/mol)	NRTL Alpha
UNIQUAC	PR kij	UNIQUAC A12 (K)	UNIQUAC A21 (K)	Not used
Chao-Seader	Not used	Not used	Not used	Not used
Grayson-Streed	Not used	Not used	Not used	Not used
Lee-Kesler-Plöcker	LKP kij	Not used	Not used	Not used
Raoult's Law	Not used	Not used	Not used	Not used
IAPWS-IF97 Steam Tables	Not used	Not used	Not used	Not used

Property Identifiers and Units

The following tables show the property identifiers and their units of measure as returned by the library. The tables were copied directly from the CAPE-OPEN Thermo 1.1 standard document. **Please note that not all properties are implemented in DTL** – if you ask for a property that is not available, a *NotImplemented* exception will be thrown by the library.

Single compound constant properties

Identifier	meaning	units
acentricFactor	Pitzer acentric factor	
associationParameter	association-parameter (Hayden-O'Connell)	
bornRadius		m
charge		
criticalCompressibilityFactor	critical compressibility factor Z	
criticalDensity	critical density	mol/m^3
criticalPressure	critical pressure	Pa
criticalTemperature	critical temperature	K
criticalVolume	critical volume	m^3/mol
diffusionVolume	diffusion volume	m^3
dipoleMoment	dipole moment	Cm
energyLennardJones	Lennard-Jones energy parameter (divided by Boltzmann constant)	K
gyrationRadius	radius of gyration	m
heatOfFusionAtNormalFreezingPoint	enthalpy change on melting at normal freezing point (101325 Pa)	J/mol
heatOfVaporizationAtNormalBoilingPoint	enthalpy change on vaporization at normal boiling point (101325 Pa)	J/mol
idealGasEnthalpyOfFormationAt25C		J/mol
idealGasGibbsFreeEnergyOfFormationAt25C		J/mol
liquidDensityAt25C	liquid density at 25 °C	mol/m^3
liquidVolumeAt25C	liquid volume at 25 °C	m^3/mol
lengthLennardJones	Lennard-Jones length parameter	m
molecularWeight	relative molar mass	
normalBoilingPoint	boiling point temperature at 101325 Pa	K
normalFreezingPoint	melting point temperature at 101325 Pa	K
parachor	Parachor	m^3 kg$^{0.25}$/(s$^{0.5}$ mol)

Identifier	meaning	units
standardEntropyGas	Standard entropy of gas	J/mol
standardEntropyLiquid	standard entropy of liquid	J/mol
standardEntropySolid	standard entropy of solid	J/mol
standardEnthalpyAqueousDilution	Standard aqueous infinite dilution enthalpy	J/mol
standardFormationEnthalpyGas	standard enthalpy change on formation of gas	J/mol
standardFormationEnthalpyLiquid	standard enthalpy change on formation of liquid	J/mol
standardFormationEnthalpySolid	standard enthalpy change on formation of solid	J/mol
standardFormationGibbsEnergyGas	standard Gibbs energy change on formation of gas	J/mol
standardFormationGibbsEnergyLiquid	standard Gibbs energy change on formation of liquid	J/mol
standardFormationGibbsEnergySolid	standard Gibbs energy change on formation of solid	J/mol
standardGibbsAqueousDilution	Standard aqueous infinite dilution Gibbs energy	J/mol
triplePointPressure	triple point pressure	Pa
triplePointTemperature	triple point temperature	K
vanderwaalsArea	van der Waals area	m^2/mol
vanderwaalsVolume	van der Waals volume	m^3/mol

Single compound temperature-dependent properties

Identifier	Meaning	units
cpAqueousInfiniteDilution	Heat capacity of a solute in an infinitely dilute aqueous solution.	J/(mol K)
dielectricConstant	The ratio of the capacity of a condenser with a particular substance as dielectric to the capacity of the same condenser with a vacuum for dielectric.	
expansivity	Coefficient of linear expansion for a solid: $\dfrac{1}{L}\dfrac{\partial L}{\partial T}\bigg\|$ (where L is the length) at 1 atm	1/K
fugacityCoefficientOfVapor	Fugacity coefficient of vapour on the saturation line	
glassTransitionPressure	Glass transition pressure	Pa
heatCapacityOfLiquid	Heat capacity (Cp) of liquid on the saturation line	J/(mol K)
heatCapacityOfSolid	Solid heat capacity (Cp) at 1 atm	J/(mol K)
heatOfFusion	Enthalpy change on fusion for the solid on the melting line	J/mol
heatOfSublimation	Enthalpy change on evaporation of the solid on the sublimation line	J/mol
heatOfSolidSolidPhaseTransition	Enthalpy change on phase transition	J/mol
heatOfVaporization	Enthalpy change on evaporation of the liquid on the saturation line	J/mol
idealGasEnthalpy	Enthalpy of ideal gas	J/mol
idealGasEntropy	Temperature-dependent part of entropy of ideal gas	J/(mol K)
idealGasHeatCapacity	Heat capacity (Cp) of ideal gas	J/(mol K)
meltingPressure	Pressure on melting line	Pa
selfDiffusionCoefficientGas	Self-diffusion coefficient in gas phase at 1 atm	M^2/s
selfDiffusionCoefficientLiquid	self-diffusion coefficient in liquid phase on saturation line	M^2/s
solidSolidPhaseTransitionPressure	Pressure at phase transition	Pa
sublimationPressure	Vapour pressure of solid on the sublimation line	Pa
surfaceTensionSatLiquid	Surface tension of liquid on the saturation line	N/m
thermalConductivityOfLiquid	Thermal conductivity of liquid on saturation line	W/(m K)
thermalConductivityOfSolid	Thermal conductivity of solid at 1 atm	W/(m K)
thermalConductivityOfVapor	Thermal conductivity of dilute gas	W/(m K)

Identifier	Meaning	units
vaporPressure	Vapour pressure of saturated liquid	Pa
virialCoefficient	Second virial coefficient of gas	M^3/mol
viscosityOfLiquid	Viscosity of liquid on saturation line	Pas
viscosityOfVapor	Viscosity in dilute gas state	Pas
volumeChangeUponMelting	Volume change for the solid on the melting line	m^3/mol
volumeChangeUponSolidSolidPhaseTransition	Volume change upon solid-solid phase transition	m^3/mol
volumeChangeUponSublimation	Volume change for the solid on the sublimation line	m^3/mol
volumeChangeUponVaporization	Volume change for the liquid on the saturation line	m^3/mol
volumeOfLiquid	Volume of liquid on saturation line	m^3/mol
volumeOfSolid	Volume of solid at 1 atm	m^3/mol

Single compound pressure-dependent properties

Identifier	Meaning	units
boilingPointTemperature	Temperature at liquid-vapour transition	K
glassTransitionTemperature	Glass transition temperature	K
meltingTemperature	Temperature on melting line	K
solidSolidPhaseTransitionTemperature	Temperature at phase transition	K

Non-constant single-phase mixture properties

Identifier	Meaning	type of property	dimensionality	units	basis	overall
activity	Activity	I	1		U	
activityCoefficient	Activity coefficient	I	1		U	
compressibility	Isothermal compressibility $\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$	I		1/Pa	U	
compressibilityFactor	Compressibility factor $Z = \frac{PV}{NRT}$	I			U	Y
density	Density	I		mol/m^3	mole/mass	Y
diffusionCoefficient	Binary diffusion coefficients for all species in mixture relative to all other species	I	2	m^2/s	U	
dissociationConstant	Chemical equilibrium constant corresponding to a dissociation reaction.	I			U	
enthalpy	Enthalpy (may or may not include the enthalpy of formation)	E		J	mole/mass	Y
enthalpyF	Enthalpy, including the enthalpy of formation	E		J	mole/mass	Y
enthalpyNF	Enthalpy, not including the enthalpy of formation	E		J	mole/mass	Y
entropy	Entropy (may or may not include the entropy of formation)	E		J/K	mole/mass	Y
entropyF	Entropy, including the entropy of formation	E		J/K	mole/mass	Y
entropyNF	Entropy, not including the entropy of formation	E		J/K	mole/mass	Y
excessEnthalpy	Excess enthalpy	E		J	mole/mass	
excessEntropy	Excess entropy	E		J/K	mole/mass	
excessGibbsEnergy	Excess Gibbs energy	E		J	mole/mass	

Identifier	Meaning	type of property	dimensionality	units	basis	overall
excessHelmholtzEnergy	Excess Helmholtz energy	E		J	mole/mass	
excessInternalEnergy	Excess internal energy	E		J	mole/mass	
excessVolume	Excess volume	E		m^3	mole/mass	
flow	Flows of each Compound in a given Phase (or the overall mixture)	E	1	mol/s	mole/mass	Y
fraction	Molar (or mass) fractions of each Compound in a given Phase (or the overall mixture)	I	1		mole/mass	Y
fugacity	Fugacity	I	1	Pa	U	
fugacityCoefficient	Fugacity coefficient	I	1		U	
gibbsEnergy	Gibbs energy	E		J	mole/mass	Y
heatCapacityCp	Heat capacity at constant pressure (Cp)	E		J/K	mole/mass	Y
heatCapacityCv	Heat capacity at constant volume (Cv)	E		J/ K	mole/mass	Y
helmholtzEnergy	Helmholtz energy	E		J	mole/mass	Y
internalEnergy	Internal energy	E		J	mole/mass	Y
jouleThomsonCoefficient	$\left(\dfrac{\partial T}{\partial P}\right)_H$	I		K/Pa	U	
logFugacity	Natural logarithm of fugacity (expressed in Pa)	I	1		U	
logFugacityCoefficient	Natural logarithm of fugacity coefficient	I	1		U	
meanActivityCoefficient	The geometrical mean of the activity coefficients of the ions in an electrolyte solution.	I	1		U	
molecularWeight	Mixture average molecular weight (relative molar mass)	I			U	

Identifier	Meaning	type of property	dimensionality	units	basis	overall
osmoticCoefficient	A measure of water activities, defined as, $\phi = -\,n_W \ln (x_W\, f_W)/(n_S\, \Sigma\nu_i)$ where, n_W is the moles of water; n_S is the moles of solute; x_W is the mole fraction of water; f_W is the symmetric activity coefficient of water; ν_I is the stoichiometric coefficient of component i.	I			U	
pH	pH	I			U	
pOH	pOH	I			U	
phaseFraction	The molar (or mass) fraction of the fluid that is in the specified phase	I			mole/mass	
pressure	Pressure	I		Pa	U	Y
speedOfSound	Thermodynamic speed of sound w, where $w^2 = (C_p / C_v)(v / M\beta_T)$ see [13]	I		m/s	U	
temperature	Temperature	I		K	U	Y
thermalConductivity	Thermal conductivity	I		W/(m K)	U	
totalFlow	Matter flow of a Phase or the overall mixture	E		mol/s	mole/mass	Y
viscosity	Viscosity	I		Pa s	U	
volume	Volume	E		m^3	mole/mass	Y