

This worksheet demonstrates the functions defined in the CoolProp user function (CoolPropMathcadWrapper.dll). CoolProp is an open-source, cross-platform, thermophysical fluid properties library developed by lan Bell et al. at the University of Liege, Liege, Belgium. The following URL provides full documentation of the CoolProp code: <a href="http://www.coolprop.org">http://www.coolprop.org</a>

# **Revision History**

2013-10-04: Creation and initial release of the CoolProp Mathcad Wrapper library. S. Polak

2013-11-01: Incorporated CoolProp 4.0.0 pre-release code . S. Polak

2016-04-30: CoolProp Function name changes for CoolProp 5.x and 6.x - J.P. Henning

2016-05-07: Added low-level functions for get fluid param string and set reference state - J.P. Henning

# Function Explanation & Examples

# **CoolProp Function Implementation Summary**

The following low-level and high-level CoolProp functions are implemented in this Mathcad wrapper:

get\_global\_param\_string("Property")
get\_fluid\_param\_string("Fluid", "Property")
set\_reference\_state("Fluid", "StateString")
PropsSI("OutProp", "InProp1", Value1, "InProp2", Value2, "Fluid")
Props1SI("Fluid", "PropName")
HAPropsSI("OutProp", "InProp1", Value1, "InProp2", Value2, , "InProp3", Value3)

Extracts global CoolProp information Extracts fluid specific information Sets the reference state for a fluid State-dependent Properties State-independent Properties Humid Air Properties

These functions will be explained in detail below and demonstrated with examples.

#### **Low Level Information Functions**

The function <code>get\_global\_param\_string</code> is a wrapper for the CoolProp low level function <code>get\_global\_param\_string()</code>. It can be used to extract parameter strings from the CoolProp library, such as the CoolProp version, error messages, and the list of fluids in the library using their acceptable name strings. Functions to parse the output of <code>get\_global\_param\_string</code> are below (hidden for clarity - click the plus symbol in the left margin to expand the hidden/collapsed area).

The parameter "version" will output a single string identifying the version of CoolProp currently installed in the Mathcad installation directory under CustomFunctions.

Current version of the CoolProp library

The function parameter "FluidsList" will output a single string representing all the fluids available in the CoolProp library. For clarity, the string parsing functions defined above (hidden by default) splits that single string into a vector of strings, providing the scrollable list of fluids as shown below:

$$strSplit \\ \\ (\texttt{get\_global\_param\_string} \\ \\ ("FluidsList") \\ \\ , ",") =$$

```
"1-Butene"
"Acetone"
"Air"
"Ammonia"
"Argon"
"Benzene"
:
```

Click on the output vector (table) to the left to enable scrolling through the entire list The parameter "predefined\_mixtures" will output a single string representing all the predefined fluid mixtures available.

The function <code>get\_fluid\_param\_string</code> is a wrapper for the CoolProp low level function <code>get\_fluid\_param\_string()</code>. It can be used to extract information from the CoolProp library about a specific to a fluid such as the aliases, Chemical Abstract Service (CAS) registry number for that fluid, the (ASHRAE) standard 34 safety rating, the equivalent REFPROP\_name, or a "pure" flag identifying if the fluid is a pure substance (true) or a mixture (false). Examples of the usage of <code>get\_fluid\_param\_string</code> are shown below:

### Aliases using the parameter "aliases"

```
get_fluid_param_string("1-Butene", "aliases")="1Butene, 1BUTENE, 1-BUTENE, Butene" get fluid param string("CO2", "aliases")="R744, co2, CO2, carbondioxide, CARBONDIOXIDE"
```

#### CAS numbers using the parameter "CAS"

```
get_fluid_param_string("1-Butene", "CAS") = "106-98-9"
get_fluid_param_string("Benzene", "CAS") = "71-43-2"
```

# ASHRAE standard 34 safety rating using the parameter "ASHRAE34"

```
get_fluid_param_string("H2", "ASHRAE34") = "A3"
get_fluid_param_string("CO2", "ASHRAE34") = "A1"
```

# REFPROP equivalent name using the parameter "REFPROPName"

```
get_fluid_param_string ("H2", "REFPROPName") = "HYDROGEN"
get_fluid_param_string ("CO2", "REFPROPName") = "CO2"
```

# Pure fluid flag using the parameter "pure"

```
get_fluid_param_string ("air", "pure") = "false"

Indicates that "air" is not a pure fluid, but a mixture.

get_fluid_param_string ("CO2", "pure") = "true"

Indicates that "CO2" is a pure fluid, not a mixture.
```

# **State Dependent Fluid Properties**

The function **PropsSI** is used to extract state-dependent fluid properties. The calling structure of the function is as follows:

```
PropsSI(Output Property <string>,
Input1 Property <string>,
Input1 Value <scalar>,
Input2 Property <string>,
Input2 Value <scalar>,
Fluid <string>)
```

Where "Fluid" is one of the fluid names from the FluidList table extracted above, and output and input properties are taken from the partial list of most common parameters below:

		Input/		
Parameter	Units	Output	Trivial	Description [units]
D, DMASS, Dmass	kg/m³	IO	False	Mass density
H, HMASS, Hmass	J/kg	IO	False	Mass specific enthalpy
Р	Pa	IO	False	Pressure
Q	mol/mol	IO	False	Mass vapor quality
S, SMASS, Smass	J/kg/K	IO	False	Mass specific entropy
Т	K	IO	False	Temperature
U, UMASS, Umass	J/kg	IO	False	Mass specific internal energy
ACENTRIC, acentric		0	True	Acentric factor
A, speed_of_sound	m/s	0	False	Speed of sound
CONDUCTIVITY, L, conductivity	W/m/K	0	False	Thermal conductivity
CPMASS, Cpmass, C	J/kg/K	0	False	Mass specific constant pressure specific heat
CVMASS, Cvmass, O	J/kg/K	0	False	Mass specific constant volume specific heat
GAS_CONSTANT,	J/mol/K	0	True	Molar gas constant
gas constant				-
I, SURFACE_TENSION	l, N/m	0	False	Surface tension
surface_tension				
M, MOLARMASS,	kg/mol	0	True	Molar mass
molarmass,				
PCRIT, P_CRITICAL,	Pa	0	True	Pressure at the critical point
Pcrit, p_critical, pcrit	t			
PMAX, P_MAX,	Pa	0	True	Maximum pressure limit
PMIN, P_MIN,	Pa	0	True	Minimum pressure limit
PRANDTL, Prandtl	[-]	0	False	Prandtl number
PTRIPLE, P_TRIPLE,	Pa	0	True	Pressure at the triple point (pure only)
p_triple, ptriple				
RHOCRIT, rhocrit	kg/m³	0	True	Mass density at critical point
TCRIT, Tcrit	K	0	True	Temperature at the critical point
TMAX, T_MAX,	K	0	True	Maximum temperature limit
T_max, Tmax				
TMIN, T_MIN,	K	0	True	Minimum temperature limit
T_min, Tmin				
TTRIPLE, T_TRIPLE,	K	0	True	Temperature at the triple point
T_triple, Ttriple				
T_FREEZE, T_freeze	K	0	True	Freezing temperature for incompressible solutions
V, VISCOSITY,	Pa s	0	False	Viscosity
viscosity				
Z	[-]	0	False	Compressibility factor ( = PV/RT)
	= =			• • • • • • • • • • • • • • • • • • • •

For a full list of valid Property parameters, please see

http://www.coolprop.org/coolprop/HighLevelAPI.html#table-of-string-inputs-to-propssi-function

# **Examples**

$$h := \text{PropsSI}(\text{"H"}, \text{"T"}, 300, \text{"P"}, 500, \text{"Helium"}) = 1563094.4$$

Enthalpy of Helium [J/kg] at a temperature of 300 K and a Pressure of 500 Pa.

PropsSI ("T", "H", 
$$h$$
, "P", 500, "Helium") = 300

Using h and 500 Pa as the input pair, the input temperature above should be returned in [K].

PropsSI 
$$\left(\text{"V"}, \text{"T"}, \frac{21 \, {}^{\bullet}C}{K}, \text{"P"}, \frac{14.7 \, {}^{\bullet}psi}{Pa}, \text{"Water"}\right) = 0.000978$$

Dynamic viscosity of Water [Pa\*s] at a temperature of 21 °C (converted to the CoolProp temperature units, K) and a Pressure of 14.7 psi (converted to the CoolProp pressure units, Pa)

# Saturated Liquid / Vapor examples

Properties along the saturation curve can be evaluated using just one of the state variables (i.e. *T*, *P*, etc.) and the vapor quality, Q, with a value of 0 for liquid, or 1 for vapor.

PropsSI 
$$\left( \text{"T", "P", } \frac{10 \text{ } MPa}{Pa}, \text{"Q", } 0, \text{"Water"} \right) = 584.147$$

Saturation temperature [K] of Water at a pressure of 10 MPa and a Quality of 0 (which is arbitrary for temperature output).

PropsSI 
$$\left( \text{"D", "P", } \frac{10 \text{ } MPa}{Pa}, \text{"Q", } 0, \text{"Water"} \right) = 688.424$$

Saturated liquid density [kg/m³] of Water at a pressure of 10 MPa.

PropsSI 
$$\left( \text{"D"}, \text{"P"}, \frac{10 \ MPa}{Pa}, \text{"Q"}, 1, \text{"Water"} \right) = 55.463$$

Saturated vapor density [kg/m³] of Water at a pressure of 10 MPa.

#### Mixture examples

Properties can be determined for a number of pre-defined mixtures; taken from the list returned by the low-level function  $get\_global\_param\_string("predefiend\_mixtures")$  as demonstrated above.

Density [kg/m³] of Air at room temperature and pressure.

User-defined mixtures can be specified in the last argument of *PropsSI(*), The mixture is specified by specifying each *fluid[mole\_fraction]* separated by & between each fluid and mole fraction in a single string. For example, Air can be user defined using 21% O2 and 79% N2 as such:

Density [kg/m³] of Air at room temperature and pressure using the user defined mixture string.

Tertiary mixtures can be specified as well by appending another pure fluid and mole fraction to the last parameter string. To improve the mixture density calculation, Argon (Ar), the next largest component in air, can be included at the following mole fraction:

$$PropsSI("D", "T", 295.16, "P", 101325, "O2[0.20948]&N2[0.78084]&AR[0.00934]") = 1.1957$$

 $CO_2$  can be added to create a quaternary mixture and further improve the accuracy of the result:

$$PropsSI("D", "T", 295.16, "P", 101325, "O2[0.20948] \& N2[0.78084] \& AR[0.00934] \& CO2[0.000314]") = 1.1963$$

Incompressible backend - using

#### **Partial Derivatives for Single-Phase States**

For some applications, it can be useful to have access to partial derivatives of thermodynamic properties. A generalized first partial derivative has been implemented into CoolProp, which can be obtained using the **PropsSI** function by encoding the desired derivative as a string. The format of the string is "d(OF)/d(WRT)|CONSTANT".

This example uses the following partial derivative of enthalpy as an alternate method for calculation the constant pressure specific heat.

$$C_p = \frac{\partial h}{\partial T}\Big|_{P}$$

Using the above encoding for the Output Property string in PropsSI:

PropsSI ("
$$d(H)/d(T)|P"$$
, "P", 101325, "T", 300, "Water") = 4180.6357765561 [J/kg/K]

As a check, using the built-in Property Name for constant pressure specific heat, we get a value of:

PropsSI ("C", "P", 
$$101325$$
, "T",  $300$ , "Water") =  $4180.6357765561$  [J/kg/K]

Second partial derivatives can be encoded into **PropsSI** as well. This is the second derivative of the above quantity, Cp, with respect to enthalpy, H, at constant pressure:

PropsSI ("d(d(H)/d(T)|P)/d(H)|P", "P", 101325, "T", 300, "Water") = 
$$-7.7679894688 \cdot 10^{-5}$$
 [1/K]

**Warning:** This second derivative formulation is currently only valid for homogeneous (single-phase) states. Two phase derivatives are not defined, and are for many combinations, invalid.

#### **Backends**

The CoolProp formulations use the Helmholtz Equation of State (HEOS). This backend is the assumed default when specifying a fluid or mixture name. However, there are other backends that can be used within the CoolProp interface (if available) and they are specified by prefixing the fluid or mixture name with the Backend name followed by a double colon, i.e. "HEOS::".

$$PropsSI\left("D","T",500,"P",101325,"INCOMP::DowQ"\right) = 809.0655$$
Incompressible backend - using DowthermQ pure fluid.

For more information on the backends for CoolProp, please see <a href="http://www.coolprop.org">http://www.coolprop.org</a>. Note that support functions for REFPROP and Tabular Interpolation are not implemented in the Mathcad wrapper at this time.

# Fluid Properties Not Dependent on State

The function **Props1SI** is used to extract fluid-specific parameters that are not dependent on the state. The calling structure of the function is as follows:

Props1SI(Fluid <string>, PropertyName <string>)

Where "Fluid" is one of the fluid names from the FluidList table above, and "PropertyName" is one of the property name abbreviations from the table below:

Tcrit Critical temperature [K] pcrit Critical pressure [Pa] Critical density [kg/m<sup>3</sup>] rhocrit Molecular mass [kg/kmol] molemass Triple-point temperature [K] Ttriple Tmin Minimum temperature [K] ptriple Triple-point pressure [Pa] Acentric factor [-] acentric

For a full list, see the CoolProp Table of String Inputs at this address:

http://coolprop.sourceforge.net/coolprop/HighLevelAPI.html#table-of-string-inputs-to-propssi-function

All items in the table marked as Trivial (True) can be entered as a "PropertyName" into the **Props1SI** function.

### Examples, Props1SI:

Props1SI("Argon", "rhocrit") = 535.6	Extracts the critical density of Argon, in [kg/m <sup>3</sup> ]

Props 
$$1SI("CO2", "ptriple") = 5.18 \cdot 10^5$$
 Extracts the critical pressure of CO2 in [Pa]

**NOTE: Props1SI(**"FluidName", "PropertyName") is just a shortcut call to **PropsSI(**"PropertyName", "",0,"",0,""FluidName") where the two input parameters are not specified and given a value of zero. The same state-independent values can be found using **PropsSI()** as shown here:

PropsSI ("ptriple", "", 0, "", 0, "CO2") = 
$$5.18 \cdot 10^5$$
 Extracts the critical pressure of CO2 in [Pa]

PropsSI ("acentric", "", 
$$0$$
, "",  $0$ , "N2") =  $0.0372$  Extracts the acentric factor of N2 in [unitless]

# **Humid Air Fluid Properties**

The function **HAPropsSI** is used to find fluid properties of humid air. The physics behind the **HAPropsSI** function is based on the analysis in ASHRAE RP-1845, which is available online: http://rp.ashrae.biz/page/ASHRAE-D-RP-1485-20091216.pdf. It employs real gas properties for both air and water, as well as the most accurate interaction parameters and enhancement factors. RP-1845 is based largely on the IAPWS-95 formulation for the properties of water. The calling structure of the function is as follows:

HAPropsSI(OutputParameter <string>, Input1 Parameter <string>, Input1 Value <scalar>, Input2 Parameter <string>, Input2 Value <scalar>, Input3 Parameter <string>, Input3 Value <scalar>)

Where "OutputParameter" and all three Input Parameters are variables from the table below:

Parameter B	<b>Aliases</b> Twb, T wb, WetBulb	Input/Output Input/Output	<b>Description [units]</b> Wet-Bulb Temperature [K]
С	ср	Output	Mixture specific heat [J/kg dry air/K]
Cha	cp_ha	Output	Mixture specific heat [J/kg humid air/K]
D	Tdp, T_dp, DewPoint	Input/Output	Dew-Point Temperature [K]
Н	Hda, Enthalpy	Input/Output	Mixture enthalpy [J/kg dry air]
Hha		Input/Output	Mixture enthalpy [J/kg humid air]
K	k, Conductivity	Output	Mixture thermal conductivity [W/m/K]
M	Visc, mu	Output	Mixture viscosity [Pa-s]
Р		Input	Pressure [Pa]
R	RH, Relhum	Input/Output	Relative humidity in (0,1) [-]
S	Sda, Entropy	Input/Output	Mixture entropy [J/kg dry air/K]
Τ	Tdb, T_db, DryBulb	Input/Output	Dry-Bulb Temperature [K]
V	Vda	Input/Output	Mixture volume [m³/kg dry air]
Vha		Input/Output	Mixture volume [m³/kg humid air]
W	Omega, HumRat	Input/Output	Humidity Ratio [kg water/kg dry air]
Z		Output	Compressibility factor (pv/RT)

#### **Examples, HAPropsSI**

HAPropsSI ("H", "T", 298.15, "P", 101325, "R", 0.5) =  $5.042 \cdot 10^4$ Enthalpy of humid air [J/kg] at a dry-bulb temperature of 298.15 K, a Pressure of 101325 Pa, and relative humidity of 0.5

HAPropsSI ("T", "P", 101325, "H", h, "R", 1.0) = 353.336Temperature of saturated air (R=1.0) at the previous enthalphy value

Note that the humid air functions at a relative humidity of zero should give roughly the same values as Dry Air from the PropsSI function. This check can be easily demonstrated here.

 $\begin{aligned} &\text{HAPropsSI}\left(\text{"V"},\text{"T"},298.15\,,\text{"P"},101325\,,\text{"R"},0\right)^{-1} = 1.184346 & \text{[kg/m³]} \\ &\text{PropsSI}\left(\text{"D"},\text{"T"},298.15\,,\text{"P"},101325\,,\text{"air"}\right) = 1.184318 & \text{[kg/m³]} \\ &\text{HAPropsSI}\left(\text{"C"},\text{"T"},298.15\,,\text{"P"},101325\,,\text{"R"},0\right) = 1006.289371 & \text{[J/kg/K]} \\ &\text{PropsSI}\left(\text{"C"},\text{"T"},298.15\,,\text{"P"},101325\,,\text{"air"}\right) = 1006.308143 & \text{[J/kg/K]} \end{aligned}$ 

#### **Reference States**

Enthalpy and entropy are relative properties! You should always be comparing differences in enthalpy rather than absolute values of the enthalpy or entropy. That said, if can be useful to set the reference state values for enthalpy and entropy to one of a few standard values. This is done by the use of the low-level **set\_reference\_state** function, which is a wrapper for the CoolProp set reference\_stateS() function.

A number of pre-defined reference states can be used:

- % IIR: h = 200 kJ/kg, s=1 kJ/kg/K at 0C saturated liquid
- % ASHRAE: h = 0, s = 0 @ -40C saturated liquid
- % NBP: h=0, s=0 for saturated liquid at 1 atmosphere
- % DEF: Go back to the default reference state for the fluid

{ IIR = International Institute of Refrigeration } { NBP = Normal Boiling Point }

as demonstrated below.

PropsSI ("H", "T", 233.15, "Q", 0, "n-Propane") = 
$$1.051 \cdot 10^5$$

PropsSI ("H", "T", 233.15, "Q", 0, "n-Butane") =  $1.108 \cdot 10^5$ 

Using the default reference state

PropsSI ("H", "T", 233.15, "Q", 0, "n-Propane") = 
$$2.928 \cdot 10^{-11}$$

PropsSI ("H", "T", 233.15, "Q", 0, "n-Butane") = 
$$1.108 \cdot 10^5$$

Using the ASHRAE reference state

Value should be zero, or very close to it.

Note that value changed for n-Propane, as requested, but not for n-Butane.

PropsSI ("H", "T", 233.15, "Q", 0, "n-Propane") = 
$$1.051 \cdot 10^5$$

PropsSI ("H", "T", 233.15, "Q", 0, "n-Butane") = 
$$1.108 \cdot 10^5$$

Back to the default (DEF) reference state

**Warning:** The changing of the reference state should <u>only</u> be done at the very beginning of your worksheet or unexpected results may occur. It is not recommended to change the reference state during the course of making calculations as done here for demonstration purposes only. Further more, because of Mathcad's top-down calculation order, switching back and forth between reference states can lead to very unexpected results (real or apparent) and is not recommended.

# **Creating Specific Unit Functions & Plotting**

Specialized Mathcad functions can be created that simplify input and correctly handle units. For example, the above saturation temperature call can be embedded in a user defined function:

$$T_{sat}(P, fluid) := \text{PropsSI}\left(\text{"T"}, \text{"P"}, \frac{P}{Pa}, \text{"Q"}, 0, fluid\right) K$$

This new function can then be used to easily calculate saturation temperature with units applied:

$$fluid :=$$
 "Water"  $P := 10 MPa$ 

$$T_{sat}(P, fluid) = 310.997 \, {}^{\bullet}C$$

This is an extremely useful and compact way to call these functions over a range and create a plot of the results.

 $P_t := \text{Props1SI}(\text{"Water"}, \text{"ptriple"}) \cdot Pa = 611.655 Pa$ 

 $P_c := \text{Props1SI}(\text{"Water"}, \text{"pcrit"}) \cdot Pa = 22.064 \text{ }MPa$ 

 $\Delta P := \frac{P_c - P_t}{100} = 0.221 \ MPa$ 

 $P := P_t, P_t + \Delta P ... P_c$ 

Start Range at Triple Point Pressure

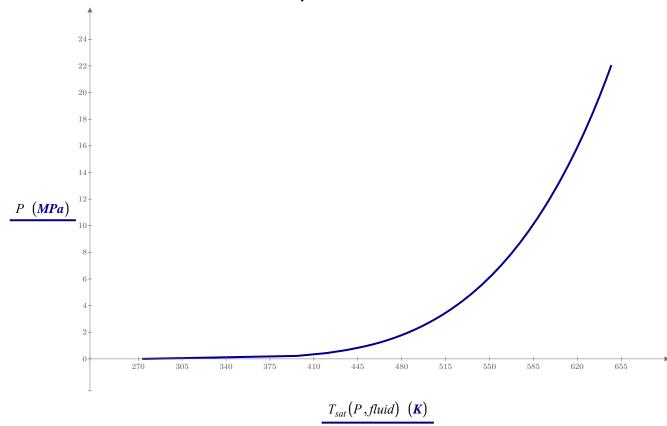
End Range at Critical Point

Pressure

Set Range Interval over 100 points

Set the Range

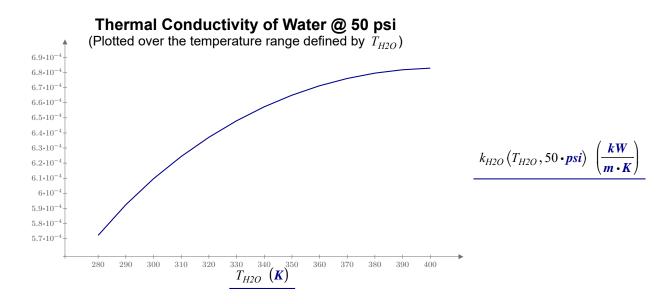
# **Plot Saturation Temperature-Pressure Curve for Water**



Unit functions of other properties can be created as well.

$$T_{H2O} := 280 \cdot K, 290 \cdot K...400 \cdot K$$

$$k_{H2O}(T, P) := \text{PropsSI}\left(\text{"L"}, \text{"T"}, \frac{T}{K}, \text{"P"}, \frac{P}{Pa}, \text{"Water"}\right) \cdot \frac{W}{m \cdot K}$$



This is an example of plotting the wet bulb temperature of humid air at various dry-bulb temperatures and relative humidity ratios, at a pressure of 1 atm.

$$T_{HA} := 290 \cdot K,300 \cdot K..370 \cdot K$$

$$T_{WB}(T, P, R) := \text{HAPropsSI}\left(\text{"B", "T", } \frac{T}{K}, \text{"P", } \frac{P}{Pa}, \text{"R", } R\right) \cdot K$$

