CoolProp IF97 Mathcad Add-in DLL Function Verification

This IF97 Mathcad Add-in DLL is based on the CoolProp imlementation of the Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (2007) and supplimentary releases for additional transport and physical properties for pure water substance. This implementation of the IF97 equations is:

- Entirely free and open-source
- Written in optimized standard C++ code so it will compile anywhere
- Fast
- Easy-to-use (just a single header)

This Mathcad worksheet provides verification of of the CoolProp IF97 imlementation and Mathcad Add-in DLL by comparing calculated values to tabulated values for computer program verification contained in the various IAPWS release documents.

IF97 Mathcad Functions

After copying the **`if97_EN.xml`** file to the directory

```
C:\Program Files (x86)\Mathcad\Mathcad 15\doc\funcdoc
```

the IF97 functions can be accessed through the Mathcad menus under **Insert | Function...**, or from the ***f(x)*** button on the toolbar. On the function panel, the IF97 functions will be under the if97 category and will all begin with the **if97_** prefix.

IF97 Thermodynamic Properties Verification for v, h, u, s, Cp, w

TP :=

T (K)	P(MPa)		
300	3	"Region 1"	"Page 9, Table 5"
300	80	"Region 1"	"Page 9, Table 5"
500	3	"Region 1"	"Page 9, Table 5"
300	0.0035	"Region 2"	"Page 17, Table 15"
700	0.0035	"Region 2"	"Page 17, Table 15"
700	30	"Region 2"	"Page 17, Table 15"
650	25.58370180	"Region 3"	"Page 32, Table 33"
650	22.29306430	"Region 3"	"Page 32, Table 33"
750	78.30956390	"Region 3"	"Page 32, Table 33"
1500	0.5	"Region 5"	"Page 40, Table 42"
1500	30	"Region 5"	"Page 40, Table 42"
2000	30	"Region 5"	"Page 40, Table 42"

$T1 := TP^{\langle 1 \rangle} \cdot K$

$kJ \equiv 1000 \cdot J$

$P1 := TP^{\langle 2 \rangle} \cdot MPa$

$i := 1 .. rows(P1)$

$j := 1 .. 6$

IF97 :=

v (m³/kg)	h (kJ/kg)	u (kJ/kg)	s (kJ/kg-K)	Cp (kJ/kg-K)	w (m/s)		
0.001002151680	115.331273	112.324818	0.392294792	4.17301218	1507.739	"Region 1"	"Page 9, Table 5"
0.000971180894	184.142828	106.448356	0.368563852	4.01008987	1634.690	"Region 1"	"Page 9, Table 5"
0.001202418000	975.542239	971.934985	2.580419120	4.65580682	1240.713	"Region 1"	"Page 9, Table 5"
39.4913866	2549.911450	2411.691600	8.522389670	1.91300162	427.9201	"Region 2"	"Page 17, Table 15"
92.3015898	3335.683750	3012.628190	10.174999600	2.08141274	644.289(	"Region 2"	"Page 17, Table 15"
0.005429466190	2631.494740	2468.610760	5.175402980	10.35050920	480.386:	"Region 2"	"Page 17, Table 15"
0.002	1863.430190	1812.262790	4.054272730	13.89357170	502.005:	"Region 3"	"Page 32, Table 33"
0.005	2375.124010	2263.658680	4.854387920	44.65793420	383.444:	"Region 3"	"Page 32, Table 33"
0.002	2258.688450	2102.069320	4.469719060	6.34165359	760.696(	"Region 3"	"Page 32, Table 33"
1.3845509	5219.768550	4527.493100	9.654088750	2.61609445	917.068(	"Region 5"	"Page 40, Table 42"
0.0230761299	5167.235140	4474.951240	7.729701330	2.72724317	928.548(	"Region 5"	"Page 40, Table 42"
0.0311385219	6571.226040	5637.070380	8.536405230	2.88569882	1067.369	"Region 5"	"Page 40, Table 42"

Verification using Newton-Raphson reverse lookup in Region 3

$$M_{i,1} := \mathrm{if97\_vtp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right) \qquad M_{i,2} := \mathrm{if97\_htp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)\frac{J}{kJ} \qquad M_{i,3} := \mathrm{if97\_utp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)\cdot\frac{J}{kJ}$$

$$M_{i,4} := \mathrm{if97\_stp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)\cdot\frac{J}{kJ} \qquad M_{i,5} := \mathrm{if97\_cptp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)\cdot\frac{J}{kJ} \qquad M_{i,6} := \mathrm{if97\_wtp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)$$

Calculate the relative error in the calculated values from the published values: $ERR_{i,j} := \frac{\left|IF97_{i,j} - M_{i,j}\right|}{IF97_{i,j}}$

Relative Error Between Calculated and Published Values

(Newton Raphson Reverse Lookup in Region 3)

ERR =

ε_v	ε_h	ε_u	ε_s	ε_{Cp}	ε_w
$3.1\cdot10^{-10}$	$1.9\cdot10^{-10}$	$1.6\cdot10^{-10}$	$1.0\cdot10^{-9}$	$9.7\cdot10^{-10}$	$2.2\cdot10^{-10}$
$2.2\cdot10^{-11}$	$1.4\cdot10^{-9}$	$2.0\cdot10^{-9}$	$1.1\cdot10^{-9}$	$8.8\cdot10^{-11}$	$1.9\cdot10^{-9}$
$2.8\cdot10^{-9}$	$10.0\cdot10^{-11}$	$9.0\cdot10^{-11}$	$2.0\cdot10^{-11}$	$4.5\cdot10^{-10}$	$2.5\cdot10^{-9}$
$9.6\cdot10^{-10}$	$3.3\cdot10^{-10}$	$9.9\cdot10^{-10}$	$3.1\cdot10^{-10}$	$5.1\cdot10^{-10}$	$6.1\cdot10^{-10}$
$1.9\cdot10^{-10}$	$1.1\cdot10^{-9}$	$2.1\cdot10^{-10}$	$2.1\cdot10^{-9}$	$1.8\cdot10^{-9}$	$6.7\cdot10^{-10}$
$8.5\cdot10^{-10}$	$1.8\cdot10^{-9}$	$4.0\cdot10^{-10}$	$4.4\cdot10^{-10}$	$8.0\cdot10^{-10}$	$3.5\cdot10^{-10}$
$4.2\cdot10^{-6}$	$1.3\cdot10^{-6}$	$1.3\cdot10^{-6}$	$1.0\cdot10^{-6}$	0.0	$8.8\cdot10^{-6}$
$1.1\cdot10^{-7}$	$2.9\cdot10^{-8}$	$2.2\cdot10^{-8}$	$2.1\cdot10^{-8}$	$4.8\cdot10^{-7}$	$4.5\cdot10^{-8}$
$1.4\cdot10^{-6}$	$3.6\cdot10^{-7}$	$4.5\cdot10^{-7}$	$3.5\cdot10^{-7}$	$1.7\cdot10^{-6}$	$1.7\cdot10^{-6}$
$8.8\cdot10^{-10}$	$2.3\cdot10^{-10}$	$4.0\cdot10^{-10}$	$3.4\cdot10^{-10}$	$1.5\cdot10^{-9}$	$3.3\cdot10^{-10}$
$2.0\cdot10^{-9}$	$1.7\cdot10^{-11}$	$3.7\cdot10^{-10}$	$4.9\cdot10^{-10}$	$8.3\cdot10^{-10}$	$2.3\cdot10^{-10}$
$9.7\cdot10^{-10}$	$2.1\cdot10^{-10}$	$4.5\cdot10^{-10}$	$1.3\cdot10^{-10}$	$4.2\cdot10^{-10}$	$1.1\cdot10^{-9}$

The largest errors are in v and Cp at 22.3 MPa and 650 K and are accurate to about 8 significant figures. These are in Region 3 where the revers lookup occurs for density. The remaining values are accurate to 8 segnificant figures or more. The verification values for Cv are not listed in the IAPWS documents.

Verification using supplimental reverse lookup equations in Region 3

Relative Error Between Calculated and Published Values

(Supplimental Reverse Lookup Functions in Region 3)

ERR =

ε_v	ε_h	ε_u	ε_s	ε_{Cp}	ε_w
$3.1\cdot10^{-10}$	$1.9\cdot10^{-10}$	$1.6\cdot10^{-10}$	$1.0\cdot10^{-9}$	$9.7\cdot10^{-10}$	$2.2\cdot10^{-10}$
$2.2\cdot10^{-11}$	$1.4\cdot10^{-9}$	$2.0\cdot10^{-9}$	$1.1\cdot10^{-9}$	$8.8\cdot10^{-11}$	$1.9\cdot10^{-9}$
$2.8\cdot10^{-9}$	$10.0\cdot10^{-11}$	$9.0\cdot10^{-11}$	$2.0\cdot10^{-11}$	$4.5\cdot10^{-10}$	$2.5\cdot10^{-9}$
$9.6\cdot10^{-10}$	$3.3\cdot10^{-10}$	$9.9\cdot10^{-10}$	$3.1\cdot10^{-10}$	$5.1\cdot10^{-10}$	$6.1\cdot10^{-10}$
$1.9\cdot10^{-10}$	$1.1\cdot10^{-9}$	$2.1\cdot10^{-10}$	$2.1\cdot10^{-9}$	$1.8\cdot10^{-9}$	$6.7\cdot10^{-10}$
$8.5\cdot10^{-10}$	$1.8\cdot10^{-9}$	$4.0\cdot10^{-10}$	$4.4\cdot10^{-10}$	$8.0\cdot10^{-10}$	$3.5\cdot10^{-10}$
$4.2\cdot10^{-6}$	$1.3\cdot10^{-6}$	$1.3\cdot10^{-6}$	$1.0\cdot10^{-6}$	0.0	$8.8\cdot10^{-6}$
$1.1\cdot10^{-7}$	$2.9\cdot10^{-8}$	$2.2\cdot10^{-8}$	$2.1\cdot10^{-8}$	$4.8\cdot10^{-7}$	$4.5\cdot10^{-8}$
$1.4\cdot10^{-6}$	$3.6\cdot10^{-7}$	$4.5\cdot10^{-7}$	$3.5\cdot10^{-7}$	$1.7\cdot10^{-6}$	$1.7\cdot10^{-6}$
$8.8\cdot10^{-10}$	$2.3\cdot10^{-10}$	$4.0\cdot10^{-10}$	$3.4\cdot10^{-10}$	$1.5\cdot10^{-9}$	$3.3\cdot10^{-10}$
$2.0\cdot10^{-9}$	$1.7\cdot10^{-11}$	$3.7\cdot10^{-10}$	$4.9\cdot10^{-10}$	$8.3\cdot10^{-10}$	$2.3\cdot10^{-10}$
$9.7\cdot10^{-10}$	$2.1\cdot10^{-10}$	$4.5\cdot10^{-10}$	$1.3\cdot10^{-10}$	$4.2\cdot10^{-10}$	$1.1\cdot10^{-9}$

The largest errors are in Region 3 where the reverse lookup occurs for density. These errors are on the order of 1E-6 using just the supplimental reverse lookup equations for density, while the error in the other regions is on the order of 1.0E-9 or lower.

Timing Test

Supplimental Reverse Lookup Functions

```
Time1 := | for j ∈ 1..100                                   = 0.028
         |   | t0 ← time(0)
         |   | for i ∈ 1..10000
         |   |   | a ← if97_vtp(T1_7/K, P1_7/Pa)
         |   |   | b ← if97_vtp(T1_8/K, P1_8/Pa)
         |   |   | c ← if97_vtp(T1_9/K, P1_9/Pa)
         |   | Δt_j ← time(0) − t0
         | mean(Δt)
```

Timing Test

Newton-Raphson Iterative Reverse Lookup

```
Time2 := | for j ∈ 1..100                                   = 0.072
         |   | t0 ← time(0)
         |   | for i ∈ 1..10000
         |   |   | a ← if97_vtp(T1_7/K, P1_7/Pa)
         |   |   | b ← if97_vtp(T1_8/K, P1_8/Pa)
         |   |   | c ← if97_vtp(T1_9/K, P1_9/Pa)
         |   | Δt_j ← time(0) − t0
         | mean(Δt)
```

Using the supplimental reverse lookup equations for density to get an accurate initial guess for pressure and then using Newton-Raphson to iterate on the original Region 3 equation increases the time to calculate denisity (specific volume) values in this region by a factor of about 2.6, but is far better than the factor of 17 indicated in the supplimental release document using an arbitrary initial guess.

Saturation Curve Verification

Set up Pressure and Temperature matrix based on tabulated values from IAPWS-IF97 on page 35, Table 36.

IAPWS Values

$$P_{IAPWS} := \begin{pmatrix} 0.1 \\ 1 \\ 10 \end{pmatrix} \cdot MPa$$

$$T_{IAPWS} := \begin{pmatrix} 372.755919 \\ 453.035632 \\ 584.149488 \end{pmatrix} \cdot K$$

$$ERR := \overrightarrow{\frac{T_{IAPWS} - T2}{T_{IAPWS}}} = \begin{pmatrix} 1.043 \times 10^{-9} \\ -8.641 \times 10^{-10} \\ 2.521 \times 10^{-12} \end{pmatrix}$$

Calculated Values

$$T2 := \overrightarrow{if97\_tsatp\left(\frac{P_{IAPWS}}{Pa}\right)} \cdot K = \begin{pmatrix} 372.756 \\ 453.036 \\ 584.149 \end{pmatrix} K$$

$$P2 := \overrightarrow{if97\_psatt\left(\frac{T_{IAPWS}}{K}\right)} \cdot Pa = \begin{pmatrix} 0.1 \\ 1 \\ 10 \end{pmatrix} \cdot MPa$$

$$ERR2 := \overrightarrow{\frac{P_{IAPWS} - P2}{P_{IAPWS}}} = \begin{pmatrix} -1.39 \times 10^{-8} \\ 9.008 \times 10^{-9} \\ -2.003 \times 10^{-11} \end{pmatrix}$$

The calculated values agree to the published values to about 8 significant figures or more.

Triple Point: $T_t := if97\_ttrip(0) \cdot K = 273.16\,K$ $\quad P_t := if97\_ptrip(0) \cdot Pa = 611.657\,Pa$

Critical Point: $T_c := if97\_tcrit(0) \cdot K = 647.096\,K$ $\quad P_c := if97\_pcrit(0) \cdot Pa = 22.064 \cdot MPa$

Set up Curve Ranges:

$$\Delta P := \frac{P_c - P_t}{1000} = 0.022 \cdot MPa \qquad \Delta T := \frac{T_c - T_t}{600} = 0.623\,K$$

$$P_s := P_t, P_t + \Delta P \,..\, P_c \qquad T_s := T_t, T_t + \Delta T \,..\, T_c$$

Saturation Functions :

$$T_{sat}(P) := round\left(if97\_tsatp\left(\frac{P}{Pa}\right), 7\right) \cdot K$$

$$P_{sat}(T) := round\left(if97\_psatt\left(\frac{T}{K}\right), 3\right) \cdot Pa$$

check :

$$T_{sat}(P_t) = 273.16\,K \qquad P_{sat}(T_t) = 611.657\,Pa$$

$$T_{sat}(P_c) = 647.096\,K \qquad P_{sat}(T_c) = 22.064 \cdot MPa$$

Region 2/3 Functions :

$T_{23}(P) := \text{if97\_t23}\left(\frac{P}{Pa}\right)\cdot K$ $\qquad P_{23}(T) := \text{if97\_p23}\left(\frac{T}{K}\right)\cdot Pa$

$T_{Bmin} := 623.15\cdot K$ $\qquad T_{Bmax} := 863.15\cdot K$

$\Delta T_B := \frac{T_{Bmax} - T_{Bmin}}{300} = 0.8\,K$ $\qquad T_B := T_{Bmin}, T_{Bmin} + \Delta T_B .. T_{Bmax}$

Region 1/3 Curve :

$T_{13_1} := T_{Bmin}$ $\qquad T_{13_2} := T_{Bmin}$

$P_{13_1} := P_{23}(T_{Bmin}) = 16.529\cdot MPa$ $\qquad P_{13_2} := 100\cdot MPa$