

CoolProp IF97 Mathcad Add-in DLL Function Verification

This IF97 Mathcad Add-in DLL is based on the CoolProp implementation of the Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (2007) and supplementary 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 the CoolProp IF97 implementation 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

These tables below contain the Reference [a] published values for verification of computer programs. Each entry shows the page number and table where the values can be found in the Reference [a] document.

	T (K)	P (MPa)				
TP :=	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"		
					$T1 := TP^{(1)} \cdot K$ $P1 := TP^{(2)} \cdot MPa$ $i := 1 \dots \text{rows}(P1)$ $j := 1 \dots 6$	$kJ \equiv 1000 \cdot J$

	v (m³/kg)	h (kJ/kg)	u (kJ/kg)	s (kJ/kg-K)	Cp (kJ/kg-K)	w (m/s)
IF97 :=	0.001002151680	115.331273	112.324818	0.392294792	4.17301218	1507.739210
	0.000971180894	184.142828	106.448356	0.368563852	4.01008987	1634.690540
	0.001202418000	975.542239	971.934985	2.580419120	4.65580682	1240.713370
	39.4913866	2549.911450	2411.691600	8.522389670	1.91300162	427.920172
	92.3015898	3335.683750	3012.628190	10.174999600	2.08141274	644.289068
	0.005429466190	2631.494740	2468.610760	5.175402980	10.35050920	480.386523
	0.002	1863.430190	1812.262790	4.054272730	13.89357170	502.005554
	0.005	2375.124010	2263.658680	4.854387920	44.65793420	383.444594
	0.002	2258.688450	2102.069320	4.469719060	6.34165359	760.696041
	1.3845509	5219.768550	4527.493100	9.654088750	2.61609445	917.068690
	0.0230761299	5167.235140	4474.951240	7.729701330	2.72724317	928.548002
	0.0311385219	6571.226040	5637.070380	8.536405230	2.88569882	1067.369480

Verification using Newton-Raphson reverse lookup in Region 3

$$M_{i,1} := \text{if97_vtp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)$$

$$M_{i,2} := \text{if97_htp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right) \frac{J}{kJ}$$

$$M_{i,3} := \text{if97_utp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right) \frac{J}{kJ}$$

$$M_{i,4} := \text{if97_stp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right) \frac{J}{kJ}$$

$$M_{i,5} := \text{if97_cptp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right) \frac{J}{kJ}$$

$$M_{i,6} := \text{if97_wtp}\left(\frac{T1_i}{K}, \frac{P1_i}{Pa}\right)$$

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

Relative Error Between Calculated and Published Values (Newton Raphson Reverse Lookup in Region 3)

	ϵ_v	ϵ_h	ϵ_u	ϵ_s	ϵ_{Cp}	ϵ_w
ERR =	$3.1 \cdot 10^{-10}$	$1.9 \cdot 10^{-10}$	$1.6 \cdot 10^{-10}$	$1.0 \cdot 10^{-9}$	$9.7 \cdot 10^{-10}$	$2.2 \cdot 10^{-10}$
	$2.2 \cdot 10^{-11}$	$1.4 \cdot 10^{-9}$	$2.0 \cdot 10^{-9}$	$1.1 \cdot 10^{-9}$	$8.8 \cdot 10^{-11}$	$1.9 \cdot 10^{-9}$
	$2.8 \cdot 10^{-9}$	$10.0 \cdot 10^{-11}$	$9.0 \cdot 10^{-11}$	$2.0 \cdot 10^{-11}$	$4.5 \cdot 10^{-10}$	$2.5 \cdot 10^{-9}$
	$9.6 \cdot 10^{-10}$	$3.3 \cdot 10^{-10}$	$9.9 \cdot 10^{-10}$	$3.1 \cdot 10^{-10}$	$5.1 \cdot 10^{-10}$	$6.1 \cdot 10^{-10}$
	$1.9 \cdot 10^{-10}$	$1.1 \cdot 10^{-9}$	$2.1 \cdot 10^{-10}$	$2.1 \cdot 10^{-9}$	$1.8 \cdot 10^{-9}$	$6.7 \cdot 10^{-10}$
	$8.5 \cdot 10^{-10}$	$1.8 \cdot 10^{-9}$	$4.0 \cdot 10^{-10}$	$4.4 \cdot 10^{-10}$	$8.0 \cdot 10^{-10}$	$3.5 \cdot 10^{-10}$
	$6.0 \cdot 10^{-10}$	$9.6 \cdot 10^{-11}$	$1.9 \cdot 10^{-9}$	$9.7 \cdot 10^{-10}$	$6.3 \cdot 10^{-9}$	$1.7 \cdot 10^{-9}$
	$1.6 \cdot 10^{-8}$	$5.9 \cdot 10^{-9}$	$1.6 \cdot 10^{-9}$	$3.1 \cdot 10^{-9}$	$6.9 \cdot 10^{-8}$	$6.0 \cdot 10^{-9}$
	$1.4 \cdot 10^{-10}$	$2.0 \cdot 10^{-9}$	$1.1 \cdot 10^{-9}$	$8.1 \cdot 10^{-10}$	$9.2 \cdot 10^{-10}$	$3.2 \cdot 10^{-10}$
	$8.8 \cdot 10^{-10}$	$2.3 \cdot 10^{-10}$	$4.0 \cdot 10^{-10}$	$3.4 \cdot 10^{-10}$	$1.5 \cdot 10^{-9}$	$3.3 \cdot 10^{-10}$
	$2.0 \cdot 10^{-9}$	$1.7 \cdot 10^{-11}$	$3.7 \cdot 10^{-10}$	$4.9 \cdot 10^{-10}$	$8.3 \cdot 10^{-10}$	$2.3 \cdot 10^{-10}$
	$9.7 \cdot 10^{-10}$	$2.1 \cdot 10^{-10}$	$4.5 \cdot 10^{-10}$	$1.3 \cdot 10^{-10}$	$4.2 \cdot 10^{-10}$	$1.1 \cdot 10^{-9}$

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 reverts lookup occurs for density. The remaining values are accurate to 8 significant figures or more. The verification values for Cv are not listed in the IAPWS documents.

Verification using supplemental reverse lookup equations in Region 3

Relative Error Between Calculated and Published Values

(Supplemental Reverse Lookup Functions in Region 3)

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

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 supplemental reverse lookup equations for density, while the error in the other regions is on the order of 1.0E-9 or lower.

Timing Test

Supplemental Reverse Lookup Functions

```

Time1 := for j ∈ 1..100                                = 0.028
          | t0 ← time(0)
          | for i ∈ 1..10000
          |   | a ← if97_vtp( $\frac{T_{17}}{K}, \frac{P_{17}}{Pa}$ )
          |   | b ← if97_vtp( $\frac{T_{18}}{K}, \frac{P_{18}}{Pa}$ )
          |   | c ← if97_vtp( $\frac{T_{19}}{K}, \frac{P_{19}}{Pa}$ )
          |   | Δtj ← 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( $\frac{T_{17}}{K}, \frac{P_{17}}{Pa}$ )
          |   | b ← if97_vtp( $\frac{T_{18}}{K}, \frac{P_{18}}{Pa}$ )
          |   | c ← if97_vtp( $\frac{T_{19}}{K}, \frac{P_{19}}{Pa}$ )
          |   | Δtj ← time(0) - t0
          | mean(Δt)

```

Using the supplemental 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 density (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 supplemental release document using an arbitrary initial guess.

Region 3 Supplemental Reverse Functions Verification

The tables below contain the Reference [b] published values for verification of computer programs. These values can be found in Table 5 (page 13) and Table 13 (page 20) of Reference [b].

$$\begin{aligned}
 R1 &:= \begin{pmatrix} 50 & 630 & 1.470853100 \\ 80 & 670 & 1.503831359 \\ 50 & 710 & 2.204728587 \\ 80 & 750 & 1.973692940 \\ 20 & 630 & 1.761696406 \\ 30 & 650 & 1.819560617 \\ 26 & 656 & 2.245587720 \\ 30 & 670 & 2.506897702 \\ 26 & 661 & 2.970225962 \\ 30 & 675 & 3.004627086 \\ 26 & 671 & 5.019029401 \\ 30 & 690 & 4.656470142 \\ 23.6 & 649 & 2.163198378 \\ 24 & 650 & 2.166044161 \\ 23.6 & 652 & 2.651081407 \\ 24 & 654 & 2.967802335 \\ 23.6 & 653 & 3.273916816 \\ 24 & 655 & 3.550329864 \\ 23.5 & 655 & 4.545001142 \\ 24 & 660 & 5.100267704 \end{pmatrix} \\
 R2 &:= \begin{pmatrix} 23 & 660 & 6.109525997 \\ 24 & 670 & 6.427325645 \\ 22.6 & 646 & 2.117860851 \\ 23 & 646 & 2.062374674 \\ 22.6 & 648.6 & 2.533063780 \\ 22.8 & 649.3 & 2.572971781 \\ 22.6 & 649 & 2.923432711 \\ 22.8 & 649.7 & 2.913311494 \\ 22.6 & 649.1 & 3.131208996 \\ 22.8 & 649.9 & 3.221160278 \\ 22.6 & 649.4 & 3.715596186 \\ 22.8 & 650.2 & 3.664754790 \\ 21.1 & 640 & 1.970999272 \\ 21.8 & 643 & 2.043919161 \\ 21.1 & 644 & 5.251009921 \\ 21.8 & 648 & 5.256844741 \\ 19.1 & 635 & 1.932829079 \\ 20 & 638 & 1.985387227 \\ 17 & 626 & 8.483262001 \\ 20 & 640 & 6.227528101 \end{pmatrix} \\
 R3 &:= \begin{pmatrix} 21.5 & 644.6 & 2.268366647 \\ 22 & 646.1 & 2.296350553 \\ 22.5 & 648.6 & 2.832373260 \\ 22.3 & 647.9 & 2.811424405 \\ 22.15 & 647.5 & 3.694032281 \\ 22.3 & 648.1 & 3.622226305 \\ 22.11 & 648 & 4.528072649 \\ 22.3 & 649 & 4.556905799 \\ 22 & 646.84 & 2.698354719 \\ 22.064 & 647.05 & 2.717655648 \\ 22 & 646.89 & 3.798732962 \\ 22.064 & 647.15 & 3.701940010 \end{pmatrix}
 \end{aligned}$$

Combine columns and split out p , T , and v .

Rev := stack(R1, R2, R3)

$P_{rev} := Rev^{(1)} \cdot \text{MPa}$ $T_{rev} := Rev^{(2)} \cdot \text{K}$

$v_{rev} := Rev^{(3)} \cdot 10^{-3}$

$j := 1 \dots \text{length}(v_{rev})$

Calculate the specific volumes using the IF97 supplemental reverse functions:

$$v'_{rev,j} := \text{if97_vtp}\left(\frac{T_{rev,j}}{\text{K}}, \frac{P_{rev,j}}{\text{Pa}}\right)$$

Relative Error

$$\epsilon_{rev} := \frac{v_{rev} - v'_{rev}}{v_{rev}}$$

$$\text{RMS}_3 := \sqrt{\frac{\sum (v_{rev} - v'_{rev})^2}{\text{length}(v_{rev})}} = 5.257 \times 10^{-13}$$

RMS error is well below the 10 significant digits listed in the tables.

$$\text{Rev}^{(4)} := v'_{rev} \cdot 10^3$$

$$\text{Rev}^{(5)} := \epsilon_{rev}$$

<== Tack calculated values and rel. error onto table.

Rev =

	p [MPa]	T [K]	v [m ³ /kg]	v_{calc} [m ³ /kg]	$rel\ error$ [unitless]
	1	2	3	4	5
1	50	630	1.4708531	1.4708531	-7.540579442·10 ⁻¹¹
2	80	670	1.503831359	1.503831359	3.055710859·10 ⁻¹⁰
3	50	710	2.204728587	2.204728587	-2.607323165·10 ⁻¹¹
4	80	750	1.97369294	1.97369294	-6.136484297·10 ⁻¹¹
5	20	630	1.761696406	1.761696406	2.67056335·10 ⁻¹⁰
6	30	650	1.819560617	1.819560617	2.589454497·10 ⁻¹⁰
7	26	656	2.24558772	2.24558772	-1.327314827·10 ⁻¹¹
8	30	670	2.506897702	2.506897702	1.477602538·10 ⁻¹⁰
9	26	661	2.970225962	2.970225962	-1.059882133·10 ⁻¹²
10	30	675	3.004627086	3.004627086	-1.191517559·10 ⁻¹⁰
11	26	671	5.019029401	5.019029401	-8.908076031·10 ⁻¹²
12	30	690	4.656470142	4.656470142	6.751252519·10 ⁻¹¹
13	23.6	649	2.163198378	2.163198378	-1.45026183·10 ⁻¹⁰
14	24	650	2.166044161	2.166044161	2.00912682·10 ⁻¹¹
15	23.6	652	2.651081407	2.651081407	1.607421253·10 ⁻¹⁰
16	24	654	2.967802335	2.967802335	2.029112835·10 ⁻¹¹
17	23.6	653	3.273916816	3.273916816	1.958872603·10 ⁻¹¹
18	24	655	3.550329864	3.550329864	9.591066802·10 ⁻¹¹
19	23.5	655	4.545001142	4.545001142	7.714460305·10 ⁻¹¹
20	24	660	5.100267704	5.100267704	8.368087891·10 ⁻¹¹
21	23	660	6.109525997	6.109525997	1.854665487·10 ⁻¹¹
22	24	670	6.427325645	6.427325645	4.643044848·10 ⁻¹¹
23	22.6	646	2.117860851	2.117860851	1.519907637·10 ⁻¹⁰
24	23	646	2.062374674	2.062374674	-7.114438656·10 ⁻¹¹
25	22.6	648.6	2.53306378	2.53306378	-1.663922941·10 ⁻¹⁰
26	22.8	649.3	2.572971781	2.572971781	3.30216292·10 ⁻¹¹
27	22.6	649	2.923432711	2.923432711	6.168245455·10 ⁻¹³
28	22.8	649.7	2.913311494	2.913311494	-1.417358105·10 ⁻¹¹
29	22.6	649.1	3.131208996	3.131208996	-2.08418848·10 ⁻¹²
30	22.8	649.9	3.221160278	3.221160278	1.977801408·10 ⁻¹¹
31	22.6	649.4	3.715596186	3.715596186	-1.311532317·10 ⁻¹⁰
32	22.8	650.2	3.66475479	3.66475479	1.04038659·10 ⁻¹⁰
33	21.1	640	1.970999272	1.970999272	...

* These values and the RMS error above were calculated with the REGION3_ITERATE switch turned off.

Saturation Curve Verification

IAPWS Values

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

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

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

$$\text{ERR} := \frac{\overrightarrow{T_{\text{IAPWS}} - T_2}}{T_{\text{IAPWS}}} = \begin{pmatrix} 1.043 \times 10^{-9} \\ -8.641 \times 10^{-10} \\ 2.521 \times 10^{-12} \end{pmatrix}$$

Calculated Values

$$T_2 := \text{if97_tsatp}\left(\frac{P_{\text{IAPWS}}}{\text{Pa}}\right) \cdot \text{K} = \begin{pmatrix} 372.756 \\ 453.036 \\ 584.149 \end{pmatrix} \text{K}$$

$$P_2 := \text{if97_psatt}\left(\frac{T_{\text{IAPWS}}}{\text{K}}\right) \cdot \text{Pa} = \begin{pmatrix} 0.1 \\ 1 \\ 10 \end{pmatrix} \cdot \text{MPa}$$

$$\text{ERR2} := \frac{\overrightarrow{P_{\text{IAPWS}} - P_2}}{P_{\text{IAPWS}}} = \begin{pmatrix} -1.39 \times 10^{-8} \\ 9.008 \times 10^{-9} \\ -2.003 \times 10^{-11} \end{pmatrix}$$

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

Triple Point: $T_t := \text{if97_ttrip}(0) \cdot \text{K} = 273.16 \text{ K}$

$$P_t := \text{if97_ptrip}(0) \cdot \text{Pa} = 611.656 \text{ Pa}$$

Critical Point: $T_c := \text{if97_tcrit}(0) \cdot \text{K} = 647.096 \text{ K}$

$$P_c := \text{if97_pcrit}(0) \cdot \text{Pa} = 22.064 \cdot \text{MPa}$$

Set up Curve Ranges: $\Delta P := \frac{P_c - P_t}{1000} = 0.022 \cdot \text{MPa}$

$$\Delta T := \frac{T_c - T_t}{600} = 0.623 \text{ K}$$

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

$$T_s := T_t, T_t + \Delta T .. T_c$$

Saturation Functions : $T_{\text{sat}}(P) := \text{round}\left(\text{if97_tsatp}\left(\frac{P}{\text{Pa}}\right), 7\right) \cdot \text{K}$

$$P_{\text{sat}}(T) := \text{round}\left(\text{if97_psatt}\left(\frac{T}{\text{K}}\right), 3\right) \cdot \text{Pa}$$

check : $T_{\text{sat}}(P_t) = 273.1599775 \text{ K}$

$$P_{\text{sat}}(T_t) = 611.657 \text{ Pa}$$

$$T_{\text{sat}}(P_c) = 647.096 \text{ K}$$

$$P_{\text{sat}}(T_c) = 22.064 \cdot \text{MPa}$$

Region 2/3 Functions :

$$T_{23}(P) := \text{if97_t23}\left(\frac{P}{\text{Pa}}\right) \cdot \text{K} \quad P_{23}(T) := \text{if97_p23}\left(\frac{T}{\text{K}}\right) \cdot \text{Pa}$$

$$T_{B\min} := 623.15 \cdot \text{K} \quad T_{B\max} := 863.15 \cdot \text{K}$$

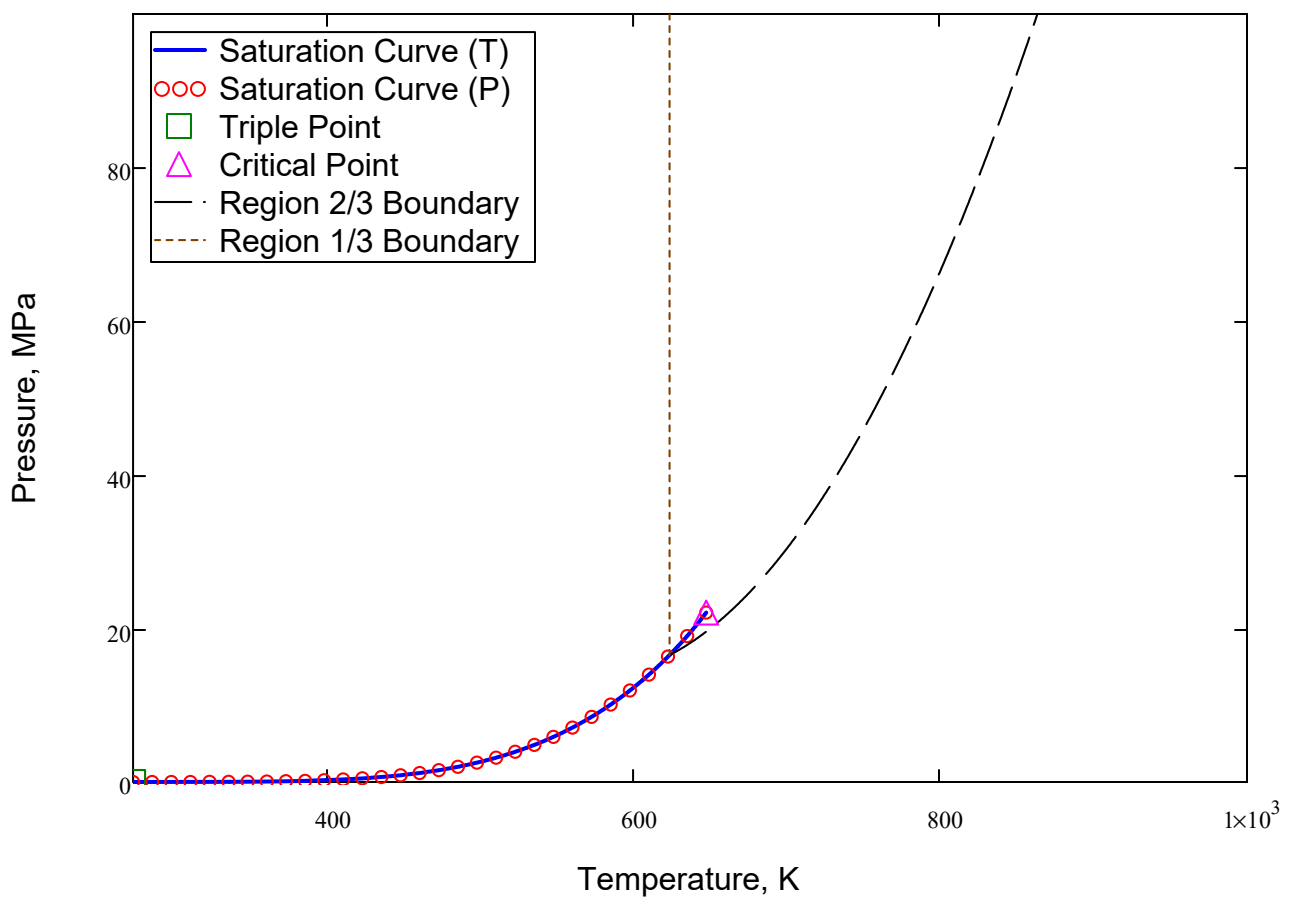
$$\Delta T_B := \frac{T_{B\max} - T_{B\min}}{300} = 0.8 \text{ K} \quad T_B := T_{B\min}, T_{B\min} + \Delta T_B \dots T_{B\max}$$

Region 1/3 Curve :

$$T_{13_1} := T_{B\min} \quad T_{13_2} := T_{B\min}$$

$$P_{13_1} := P_{23}(T_{B\min}) = 16.529 \cdot \text{MPa} \quad P_{13_2} := 100 \cdot \text{MPa}$$

Steam/Water Saturation and Boundary Curves



Saturation Function Verification and Continuity Check

Discrete Pressure Isobars

$p1 := 0.05 \cdot \text{MPa}$ $p4 := P_c$
 $p2 := .5 \cdot \text{MPa}$ $p5 := 50 \cdot \text{MPa}$
 $p3 := 5 \cdot \text{MPa}$ $p6 := 100 \cdot \text{MPa}$

Define Specific Volume Functions with Units

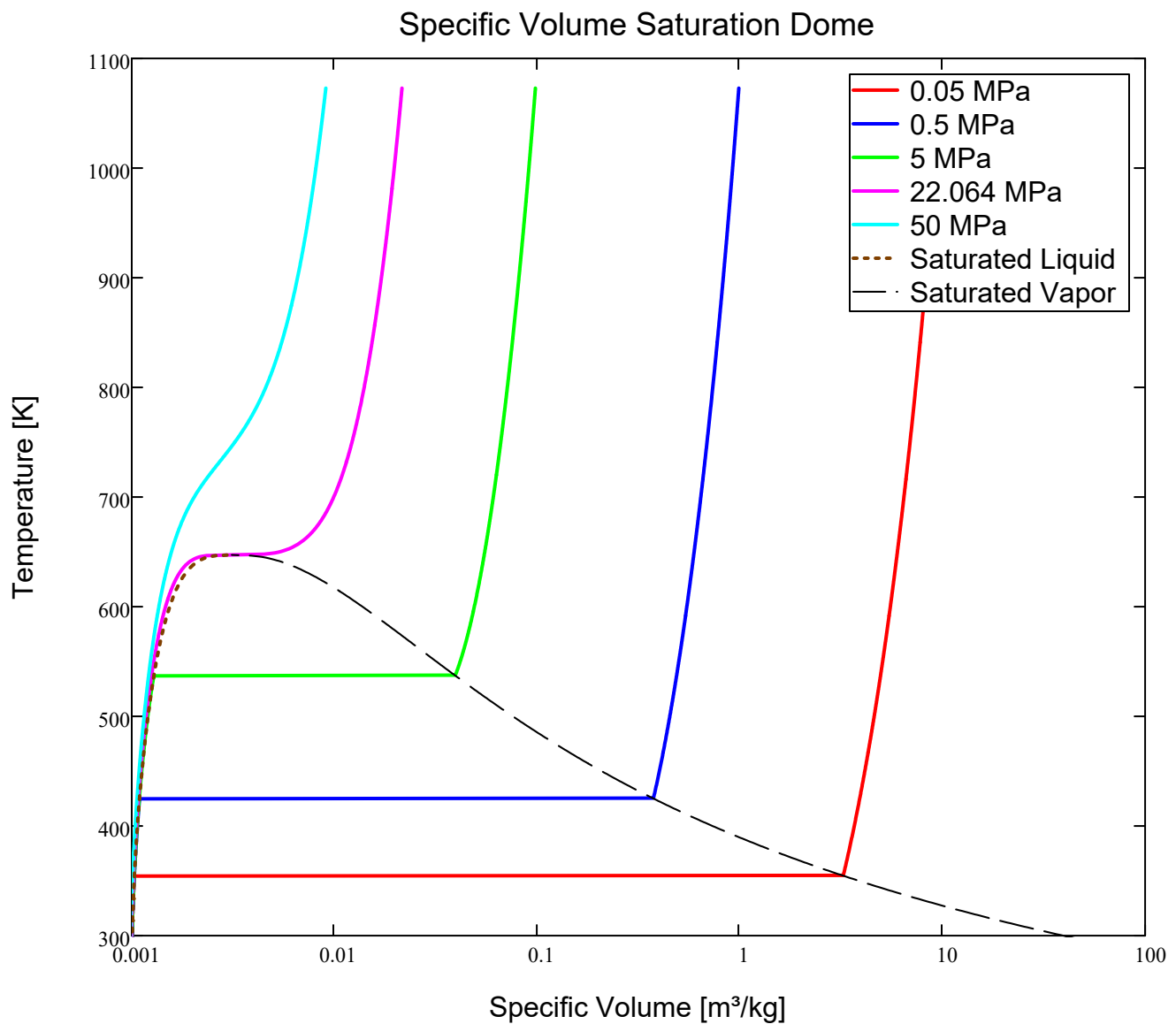
$$v_{tp}(T, P) := \text{if97_vtp}\left(\frac{T}{K}, \frac{P}{Pa}\right) \cdot \frac{\text{m}^3}{\text{kg}}$$

$$v_f(P) := \text{if97_vf}\left(\frac{P}{Pa}\right) \cdot \frac{\text{m}^3}{\text{kg}}$$

$$v_g(P) := \text{if97_vg}\left(\frac{P}{Pa}\right) \cdot \frac{\text{m}^3}{\text{kg}}$$

Temperature Range

$TT := T_t, T_t + \Delta T .. 1073.15 \cdot K$



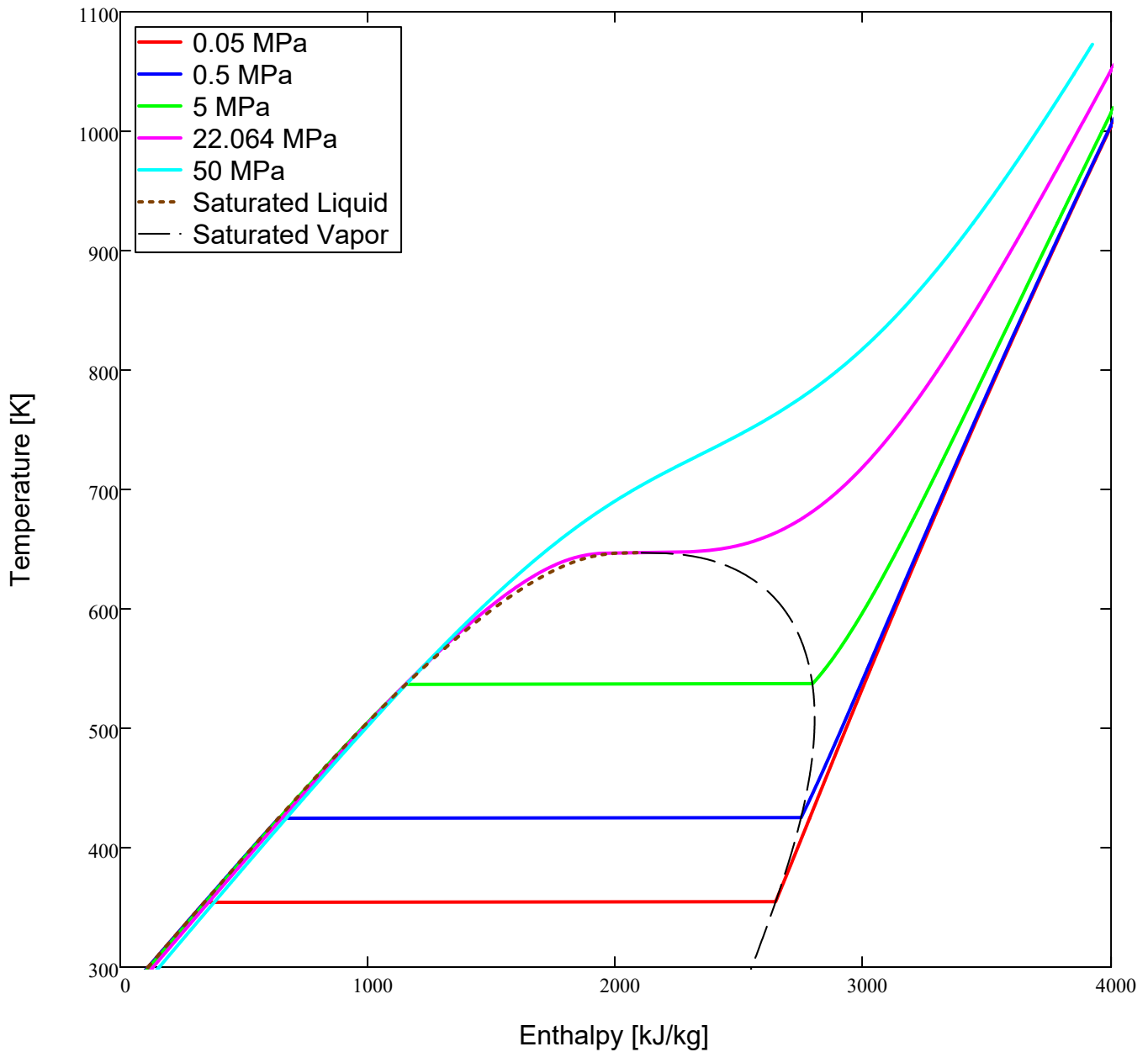
Define Enthalpy Unit Functions:

$$h_{tp}(T, P) := \text{if97_htp}\left(\frac{T}{K}, \frac{P}{Pa}\right) \cdot \frac{J}{kg}$$

$$h_f(P) := \text{if97_hf}\left(\frac{P}{Pa}\right) \cdot \frac{J}{kg}$$

$$h_g(P) := \text{if97_hg}\left(\frac{P}{Pa}\right) \cdot \frac{J}{kg}$$

Enthalpy Saturation Dome



Water Viscosity Property Verification

Set up Pressure and Temperature matrix based on tabulated values from IAPWS Reference [c], page 8, Table 4. First define: $\mu\text{Pa} \equiv 10^{-6}\text{Pa}$

Define Viscosity Unit Functions:

Saturated Liquid

Saturated Vapor

$$\mu_{\text{tp}}(T, P) := \text{if97_mutp}\left(\frac{T}{\text{K}}, \frac{P}{\text{Pa}}\right) \cdot \text{Pa} \cdot \text{s}$$

$$\mu_{\text{f}}(p) := \text{if97_muf}\left(\frac{p}{\text{Pa}}\right) \cdot \text{Pa} \cdot \text{s}$$

$$\mu_{\text{g}}(p) := \text{if97_mug}\left(\frac{p}{\text{Pa}}\right) \cdot \text{Pa} \cdot \text{s}$$

$$\mu_{\text{tp}}(T, \rho) := \text{if97_mutrho}\left(\frac{T}{\text{K}}, \frac{\rho}{\text{kg} \cdot \text{m}^{-3}}\right) \cdot \text{Pa} \cdot \text{s}$$

Function of T and ρ only set up for verification purposes

IAPWS Values

$$T_{\mu} := \begin{pmatrix} 298.15 \\ 298.15 \\ 373.15 \\ 433.15 \\ 433.15 \\ 873.15 \\ 873.15 \\ 873.15 \\ 1173.15 \\ 1173.15 \\ 1173.15 \end{pmatrix} \cdot \text{K} \quad \rho_{\mu} := \begin{pmatrix} 998 \\ 1200 \\ 1000 \\ 1 \\ 1000 \\ 1 \\ 100 \\ 600 \\ 1 \\ 100 \\ 400 \end{pmatrix} \cdot \frac{\text{kg}}{\text{m}^3} \quad \mu^* := \begin{pmatrix} 889.7351 \\ 1437.649467 \\ 307.883622 \\ 14.538324 \\ 217.685358 \\ 32.619287 \\ 35.802262 \\ 77.430195 \\ 44.217245 \\ 47.640433 \\ 64.154608 \end{pmatrix} \cdot \mu\text{Pa} \cdot \text{s}$$

Calculated Values

$$\mu_{\text{tp}}(T_{\mu}, \rho_{\mu}) = \begin{pmatrix} 889.735100 \\ 1437.649467 \\ 307.883622 \\ 14.538324 \\ 217.685358 \\ 32.619287 \\ 35.802262 \\ 77.430195 \\ 44.217245 \\ 47.640433 \\ 64.154608 \end{pmatrix} \cdot \mu\text{Pa} \cdot \text{s}$$

Relative Error from Published Values

$$\text{Err}_{\text{IAPWS}} := \left(\frac{\mu^* - \mu_{\text{tp}}(T_{\mu}, \rho_{\mu})}{\mu^*} \right) =$$

	1
1	$-1.684 \cdot 10^{-10}$
2	$2.168 \cdot 10^{-10}$
3	$-1.109 \cdot 10^{-9}$
4	$-3.341 \cdot 10^{-8}$
5	$-1.218 \cdot 10^{-9}$
6	$7.977 \cdot 10^{-10}$
7	$7.768 \cdot 10^{-9}$
8	$-2.935 \cdot 10^{-9}$
9	$1.097 \cdot 10^{-8}$
10	$-1.702 \cdot 10^{-9}$
11	$2.364 \cdot 10^{-9}$

Root Mean Square

$$\text{RMS}(M) := \sqrt{\frac{\sum_{i=1}^{\text{rows}(M)} \sum_{j=1}^{\text{cols}(M)} (M_{i,j})^2}{\text{rows}(M) \cdot \text{cols}(M)}}$$

$$\text{RMS}(\text{Err}_{\text{IAPWS}}) = 1.095 \times 10^{-8}$$

The next two tables represent the experimental data from Reference [d] (Appendix A) for water viscosity measurements [$\mu\text{Pa}\cdot\text{s}$] taken over the full IF97 range of temperatures and pressures. The data is presented here in two halves, but will be combined and extracted into matrices for comparison with the calculated values. Note that there is a typographical error in Reference [d] that printed the temperature in column fourteen in the Appendix A table as 500°C, when it should have been 450°C in the temperature series.

Appendix A-1: Table of Critically-Evaluated Experimental Data

		Temperature, °C										
		0	25	50	75	100	150	200	250	300	350	375
Pressure, Mpa	0.1	1791	890.9	547.1	377.3	12.42	14.29	16.26	18.3	20.36	22.43	23.45
	0.5	1790	891.2	546.7	378	281.7	182.3	16.05	18.16	20.25	22.32	23.43
	1	1789	891.1	546.8	378.2	281.9	182.4	15.92	18.09	20.21	22.29	23.4
	2.5	1786	890.8	547.1	378.5	282.3	182.8	134.6	17.85	20.07	22.22	23.37
	5	1780	890.3	547.7	379.2	283.1	183.4	135.2	106.5	19.88	22.15	23.33
	7.5	1774	889.8	548.3	379.8	283.8	184.1	135.9	107.2	19.75	22.12	23.34
	10	1768	889.4	548.7	380.4	284.7	184.7	136.4	107.8	87.1	22.16	23.39
	12.5	1762	889.1	549.1	381	285.3	185.3	137	108.5	88	22.35	23.57
	15	1756	888.7	549.5	381.6	286	186	137.6	109.1	89	22.84	23.88
	17.5	1750	888.5	550	382.3	286.7	186.6	138.2	109.8	89.9	67.3	24.49
	20	1744	888.2	550.4	382.9	287.4	187.3	138.8	110.4	90.8	69.5	25.85
	22.5	1738	887.9	550.9	383.5	288	187.9	139.4	111.1	91.6	71.4	48.2
	25	1733	887.6	551.3	384.2	288.7	188.5	140	111.7	92.4	73	58.8
	27.5	1728	887.4	551.8	384.8	289.4	189.1	140.6	112.3	93.1	74.4	62.4
	30	1723	887.2	552.3	385.5	290	189.8	141.2	112.9	93.9	75.7	64.9
	35	1713	886.8	553.3	386.7	291.4	191	142.3	114.1	95.3	78	68.6
	40	1705	886.6	554.3	388	292.7	192.2	143.5	115.3	96.5	79.9	71.3
	45	1697	886.5	555.3	389.3	294	193.4	144.6	116.4	97.8	81.7	73.7
	50	1690	886.4	556.3	390.6	295.4	194.6	145.8	117.6	99	83.4	75.9
	55	1684	886.5	557.4	392	296.7	195.8	146.9	118.7	100.2	84.9	77.8
	60	1679	886.7	558.5	393.3	298	197	148	119.7	101.3	86.3	79.5
	65	1674	886.9	559.7	394.6	299.4	198.2	149	120.8	102.5	87.7	81.1
	70	1670	887.3	560.9	395.9	300.7	199.4	150.1	121.9	103.6	89	82.5
	75	1666	887.7	562	397.3	302	200.6	151.2	122.9	104.6	90.3	83.9
	80	1662	888.3	563.3	398.6	303.4	201.8	152.3	123.9	105.6	91.4	85.2
	85	1659	888.8	564.5	400	304.6	203	153.3	124.9	106.6	92.6	86.4
	90	1656	889.5	565.8	401.4	305.9	204.2	154.3	125.9	107.6	93.7	87.5
	95	1653	890.3	567.1	402.8	307.3	205.4	155.4	126.9	108.6	94.7	88.7
	100	1651	891.1	568.4	404.2	308.6	206.5	156.4	127.9	109.6	95.8	89.8

Appendix A-2: Table of Critically-Evaluated Experimental Data

		Temperature, °C										
		400	425	450	475	500	550	600	650	700	750	800
Pressure, Mpa	0.1	24.47	25.49	26.5	27.51	28.52	30.53	32.55	34.6	36.6	38.6	40.5
	0.5	24.44	25.49	26.53	27.57	28.64	30.67	32.77	34.7	36.7	38.5	40.3
	1	24.43	25.49	26.53	27.58	28.65	30.68	32.79	34.8	36.8	38.5	40.4
	2.5	24.41	25.49	26.54	27.59	28.66	30.72	32.84	34.8	36.8	38.6	40.4
	5	24.42	25.52	26.6	27.66	28.73	30.82	32.77	34.9	36.9	38.7	40.6
	7.5	24.46	25.58	26.68	27.76	28.81	30.94	32.87	34.9	37	38.8	40.7
	10	24.52	25.65	26.75	27.82	28.95	31.08	33.02	35.1	37.2	39	40.9
	12.5	24.69	25.81	26.91	27.98	29.09	31.19	33.2	35.2	37.4	39.2	41.1
	15	24.98	26.06	27.13	28.18	29.3	31.44	33.4	35.5	37.6	39.4	41.2
	17.5	25.37	26.38	27.42	28.42	29.49	31.7	33.7	35.7	37.8	39.6	41.4
	20	26.03	26.83	27.8	28.76	29.81	31.98	33.9	35.9	38	39.8	41.6
	22.5	27.11	27.5	28.31	29.17	30.17	32.38	34.2	36.2	38.2	39.8	41.9
	25	29.1	28.43	28.99	29.7	30.56	32.73	34.6	36.5	38.5	40.2	41.9
	27.5	33.88	29.81	29.84	30.33	31.08	33.11	34.9	36.8	38.7	40.4	42.2
	30	43.97	31.84	30.97	31.06	31.68	33.6	35.3	37.2	39	40.7	42.5
	35	56.4	39.47	34.19	33.17	33.1	34.6	36.1	37.9	39.8	41.3	43
	40	62.1	49.26	39.16	36.06	35.2	35.7	37.5	38.8	40.4	42	43.7
	45	65.8	55.6	44.87	39.9	37.6	37.4	38.6	40	41.2	43.1	44.4
	50	68.2	60.1	50.5	44	40.5	39.1	40	40.6	42.2	43.7	45.3
	55	70.9	63.6	55.3	48.4	43.9	41	41.4	41.8	42.5	44.6	45.9
	60	73.1	66.1	59.2	52.3	47.6	43.1	41.7	42.9	43.2	44.8	46.6
	65	75.2	68.1	62.3	55.5	50.8	45.1	43.2	43.9	44.2	45.4	46.8
	70	76.9	70.5	64.9	58.8	53.7	47.5	44.8	44.3	44.4	46.2	47.4
	75	78.5	72.2	66.9	61.3	56.2	49.7	45.7	45.5	45.6	46.8	48.1
	80	79.9	74	68.3	63.6	58.7	52.1	47.4	47	46.6	47.3	48.6
	85	81.4	75.8	70.2	65.5	60.8	54	49.9	47.6	47.6	48.1	49
	90	82.7	77.2	72.3	67.3	62.8	55.8	51.4	48.9	49.1	48.9	49.7
	95	83.6	78.6	73.8	69.1	64.6	57.7	53.6	50.9	49.5	49.8	50.3
	100	85	79.8	74.6	69.8	66.1	59.3	55.1	52.1	50.5	51.1	51

$M := \text{augment}(M1, M2)$ $P_{IAPS} := \text{submatrix}(M, 2, \text{rows}(M), 1, 1) \cdot \text{MPa}$ $i := 1 \dots \text{rows}(P_{IAPS})$
 $T_{IAPS} := \text{submatrix}(M, 1, 1, 2, \text{cols}(M))^T \cdot ^\circ\text{C}$ $j := 1 \dots \text{rows}(T_{IAPS})$
 $\mu_{IAPS} := \text{submatrix}(M, 2, \text{rows}(M), 2, \text{cols}(M)) \cdot (\mu\text{Pa} \cdot \text{s})$

Calculate IF97 values:

$$\mu_{\text{calc},i,j} := \mu_{\text{tp}}(T_{\text{IAPS},j}, P_{\text{IAPS},i})$$

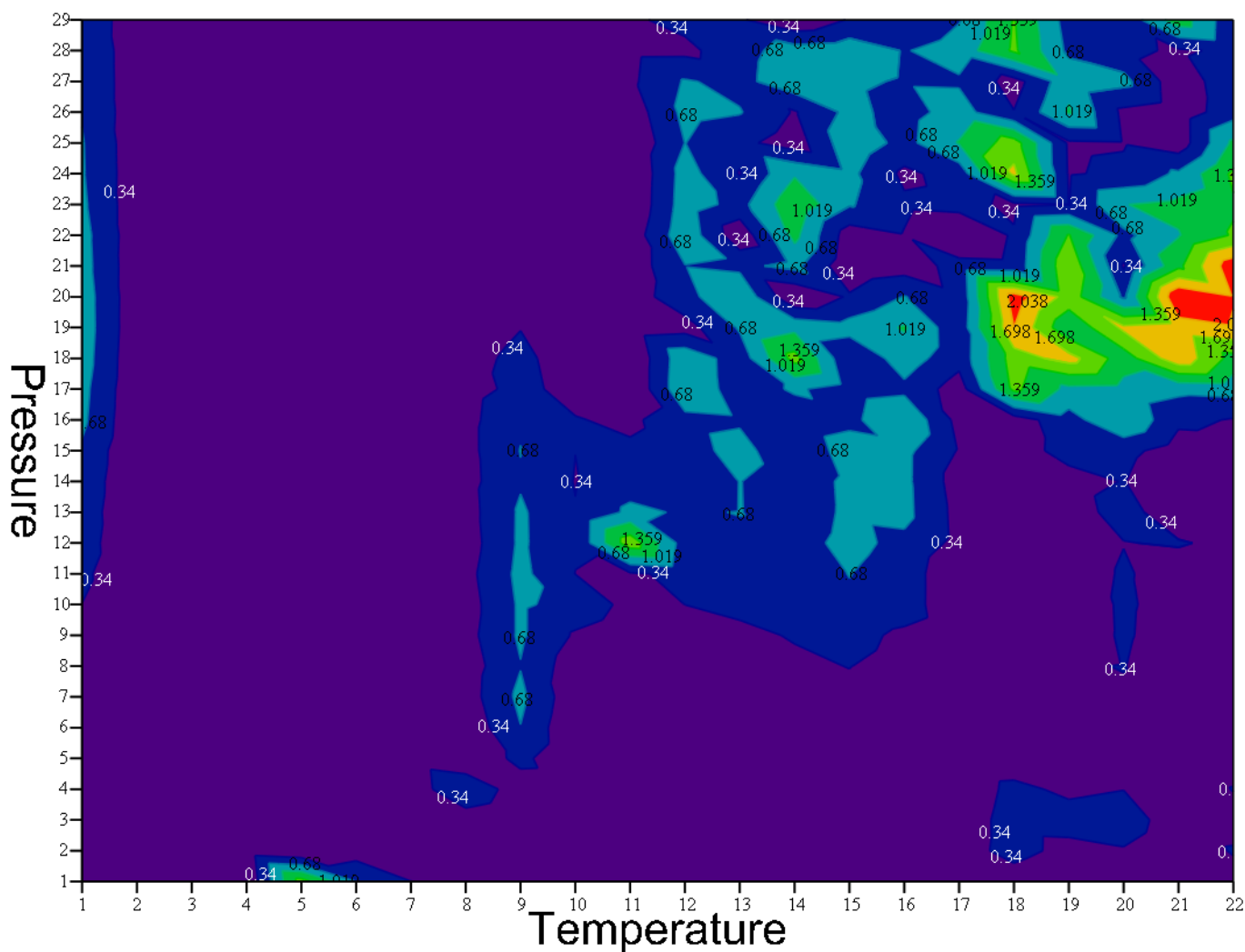
Calculate IF97 relative error:

$$\text{err}_{\text{IAPS}} := \left(\frac{|\mu_{\text{IAPS}} - \mu_{\text{calc}}|}{\mu_{\text{IAPS}} \%} \right)$$

$$\text{RMS}(\text{err}_{\text{IAPS}}) = 0.526771 \%$$

$$\max(\text{err}_{\text{IAPS}}) = 2.377 \%$$

Relative IF97 Viscosity Error (%) from IAPS Experimental Data



The RMS error is around 0.5% and the maximum relative error is about 2.4% in the high temperature, moderate pressure vapor region. This maximum occurs in an area where the measurement uncertainty is between 2.6 and 3.0%. Relative error everywhere else is predominantly well below the relative measurement uncertainty of 1.4 to 2.6%.

Water Surface Tension Verification

Set up matrix based on tabulated values from IAPWS Reference [e], pages 4-5, Table 1.

First define: $\text{mN} \equiv 0.001 \cdot \text{N}$ $\text{mN/m} \equiv \frac{\text{mN}}{\text{m}}$

$M_\sigma :=$

Temperature	Experimental σ	Uncertainty $\Delta\sigma$	Calculated σ_{calc}	Error $\sigma_{\text{calc}} - \sigma$
°C	mN/m	mN/m	mN/m	mN/m
0.01	75.64	0.38	75.65	0.01
5	74.94	0.37	74.94	0.00
10	74.23	0.37	74.22	-0.01
15	73.49	0.37	73.49	0.00
20	72.74	0.36	72.74	0.00
25	71.98	0.36	71.97	-0.01
30	71.19	0.36	71.19	0.00
35	70.41	0.35	70.40	-0.01
40	69.59	0.35	69.60	0.01
45	68.78	0.34	68.78	0.00
50	67.93	0.34	67.94	0.01
55	67.09	0.34	67.10	0.01
60	66.24	0.33	66.24	0.00
65	65.36	0.33	65.37	0.01
70	64.47	0.32	64.48	0.01
75	63.57	0.32	63.58	0.01
80	62.68	0.31	62.67	-0.01
85	61.76	0.31	61.75	-0.01
90	60.82	0.30	60.82	0.00
95	59.88	0.30	59.87	-0.01
100	58.92	0.29	58.91	-0.01
105	57.95	0.29	57.94	-0.01
110	56.97	0.28	56.96	-0.01
115	55.98	0.28	55.97	-0.01
120	54.97	0.27	54.97	0.00

$$T_\sigma := M_\sigma^{(1)} \text{ } ^\circ\text{C}$$

$$\sigma_{\text{exp}} := M_\sigma^{(2)} \cdot \text{mN/m}$$

$$\sigma_u := M_\sigma^{(3)} \cdot \text{mN/m}$$

$$\sigma_{\text{calc}} := M_\sigma^{(4)} \cdot \text{mN/m}$$

Set up a unit handling function for surface tension, $\sigma(T)$:

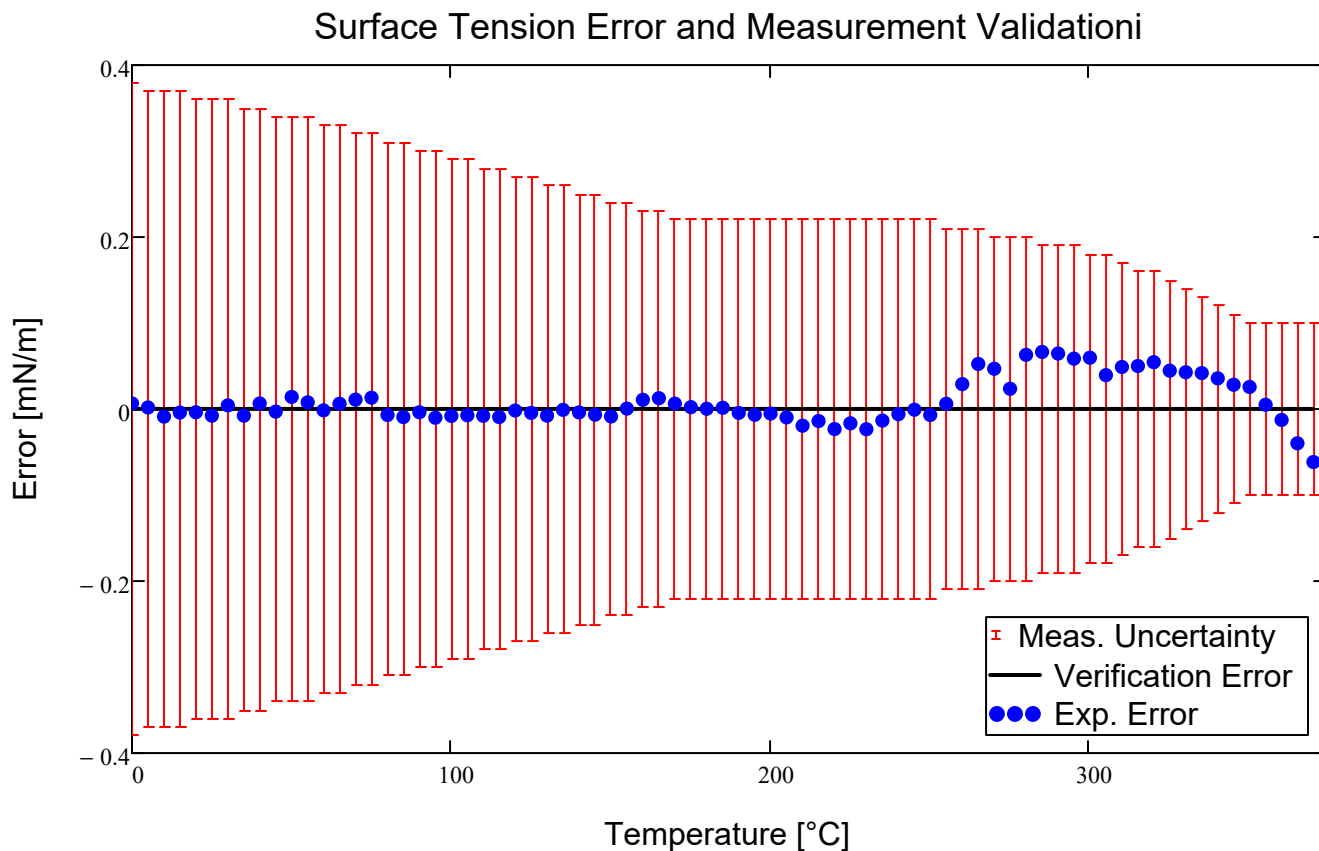
$$\sigma(T) := \text{if97_sigma}\left(\frac{T}{K}\right) \cdot \frac{N}{m}$$

Calculate error from the published verification values.

$$\varepsilon_{97} := \frac{\overrightarrow{\text{Round}(\sigma(T_\sigma), 0.01 \text{ mN/m}) - \sigma_{\text{calc}}}}{\text{mN/m}} \quad \max(\varepsilon_{97}) = 1.388 \times 10^{-14}$$

Calculate the error from the experimental values:

$$\varepsilon_\sigma := \overrightarrow{(\sigma(T_\sigma) - \sigma_{\text{exp}})}$$



The calculated values match the published values exactly to the published precision. The difference between the calculated values and the experimental measurements from IAPS data is within the measurement uncertainty of the data.

References

- [a] IAPWS, *Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, Lucerne, Switzerland, August 2007. [IAPWS R7-97(2012)]
- [b] IAPWS, *Revised Supplementary Release on Backward Equations for Specific Volume as a Function of Pressure and Temperature $v(p, T)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, Moscow, Russia, 2014. [IAPWS SR5-05(2016)]
- [c] IAPWS, *Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance*, Berlin, Germany, September 2008. [IAPWS R12-08]
- [d] IAPWS, *Revised Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance*, Vejle, Denmark, August 2003.
- [e] IAPWS, *Revised Release on Surface Tension of Ordinary Water Substance*, Moscow, Russia, June 2014. [IAPWS R1-76(2014)]