C(++)/PYTHON Library for Water-Steam Properties using the IAPWS IF97 Standard

Ling Zou, PhD

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Abstract

I would like to build a C(++)/Python library for water and steam table following the industrial formulation 1997 (IF97) standard provided by International Association for the Properties of Water and Steam (IAPWS).

Well, why am I doing this? Simply it is fun! I have seen many other such libraries built in C++, Java, and other languages. I like to write application codes with C++. However, with respect to building a library, I like pure C. It will be easier to embed such a library into applications written in other languages. Of course this project is not just for fun. I had and still having a lot of passion in two-phase flow modeling and simulation. This library will serve me well when I explore the two-phase flow world. It will always be my pleasure if you find this library useful.

1 The Saturation Line

Ideally, the saturation line should be obtained from using the Maxwell criterion for phase-equilibrium condition, see for example, Table 31 of [1]. Instead, IAPWS-IF97 [1] provides two auxiliary equations, i.e., equation (30) to compute p_{sat} from T, and (31) to compute T_{sat} from p, as its Region 4 equations. Both equations are exact solutions to an implicit quadratic equation, i.e., equation (29) of [1], and therefore are completely consistent to each other. They are valid in the range between the triple point to the critical point, while can be extrapolated to 273.15K, thus:

$$
\begin{aligned}
273.15 \text{ K} \le T \le 647.096 \text{ K} \\
611.213 \text{ Pa} \le p \le 22.064 \text{ MPa.}
\end{aligned}
$$

These two auxiliary equations are inconsistent with those based on the Maxwell criterion. As discussed in section 10.2 of IAPWS-IF97 [1], the inconsistencies are extremely small. For other properties on the saturation line, they are discussed in two segments, [273.15K, 623.15K] and [623.15K, 647.096K] in the following sections:

1.1 Segment [273.15K, 623.15K]

Saturation properties, such as the saturated water and steam densities, are directly calculated from Region 1 and 2 functions using (p, T_{sat}) or (p_{sat}, T), depending on the input parameter, p or T. For example,

$$
\begin{aligned}
T_{sat} &= T_{sat}(p) \\
\rho_{l,sat} &= \frac{1}{v_{l,sat}(p, T_{sat})} \\
\rho_{g,sat} &= \frac{1}{v_{g,sat}(p, T_{sat})}
\end{aligned}
$$

For more details, one can refer to function `genR4_sat_line()` implemented in `IF97_helper.C`.

1.2 Segment [623.15K, 647.096K]

In Region 3, properties are not expressed as functions of (p, T), so saturation properties cannot be calculated as described in section 1.1. Indeed, we have to partially rely on the Maxwell criterion, which states that, following IAPWS-IF97 [1] and its nomenclature,

$$\frac{p_s}{RT\rho'} = \delta'\phi_\delta(\delta', \tau) \tag{1}$$

$$\frac{p_s}{RT\rho''} = \delta''\phi_\delta(\delta'', \tau) \tag{2}$$

$$\frac{p_s}{RT}\left(\frac{1}{\rho''} - \frac{1}{\rho'}\right) = \phi(\delta', \tau) - \phi(\delta'', \tau) \tag{3}$$

Since p_s can be calculated from T using equation (30) of IAPWS-IF97 [1], (3) is no longer needed, and saturation densities can be solved from (1) and (2). However, one should note that equations (1) and (2) are indeed the same. For an input T, and $p_s = p_s(T)$ from equation (30) of IAPWS-IF97 [1], this equation is nonlinear and has three roots for ρ (see for example Figure 1). The two valid roots can be found using iterative numerical methods, among which bisection method is probably the most reliable one.

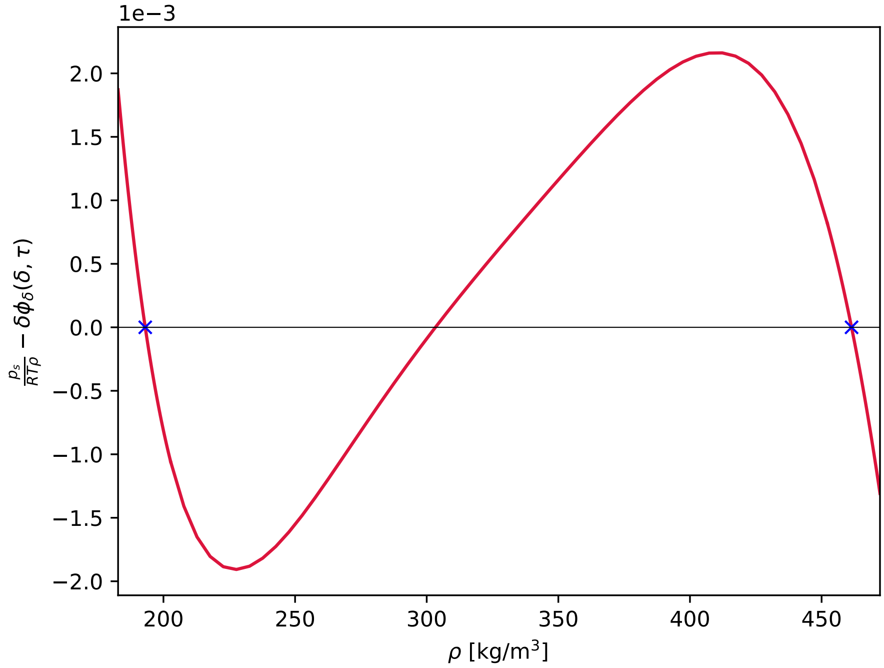

Figure 1: For an input T=642.15K, three roots can be found for $\frac{p_s}{RT\rho} = \delta\phi_\delta(\delta, \tau)$, two of which are valid. The larger one is $\rho_{l,sat}$, while the smaller one is $\rho_{g,sat}$.

2 List of Functions

Table 1: Region 1 functions list in IF97.h/C

Function Name	Function Description	Reference
`R1_gamma`	Region 1, dimensionless specific Gibbs free energy, γ	Eqn. (7) of [1]
`R1_gamma_pi`	Region 1, partial derivative, γ_π	Table 4 of [1]
`R1_gamma_tau`	Region 1, partial derivative, γ_τ	Table 4 of [1]
`R1_gamma_pi_pi`	Region 1, partial derivative, $\gamma_{\pi\pi}$	Table 4 of [1]
`R1_gamma_tau_tau`	Region 1, partial derivative, $\gamma_{\tau\tau}$	Table 4 of [1]
`R1_gamma_pi_tau`	Region 1, partial derivative, $\gamma_{\pi\tau}$	Table 4 of [1]
`R1_specific_volume`	Region 1, specific volume, v	Table 3 of [1]
`R1_specific_int_energy`	Region 1, specific internal energy, e	Table 3 of [1]
`R1_specific_entropy`	Region 1, specific entropy, s	Table 3 of [1]
`R1_specific_enthalpy`	Region 1, specific enthalpy, h	Table 3 of [1]
`R1_cp`	Region 1, specific isobaric heat capacity, c_p	Table 3 of [1]
`R1_cv`	Region 1, specific isochoric heat capacity, c_v	Table 3 of [1]
`R1_sound_speed`	Region 1, specific of sound, w	Table 3 of [1]
`R1_T_from_p_h`	Region 1, backward function $T = T(p, h)$	Eqn. (11) of [1]
`R1_T_from_p_s`	Region 1, backward function $T = T(p, s)$	Eqn. (13) of [1]

Table 2: Region 2 functions implemented in IF97.h/C

Function Name	**Function Description**	**Reference**
`R2_gamma_0`	Region 2, dimensionless specific Gibbs free energy, ideal gas part, γ^0	Eqn. (16) of [1]
`R2_gamma_r`	Region 2, dimensionless specific Gibbs free energy, residual part, γ^r	Eqn. (17) of [1]
`R2_gamma_0_pi`	Region 2, partial derivative, γ^0_π	Table 13 of [1]
`R2_gamma_0_tau`	Region 2, partial derivative, γ^0_τ	Table 13 of [1]
`R2_gamma_0_pi_pi`	Region 2, partial derivative, $\gamma^0_{\pi\pi}$	Table 13 of [1]
`R2_gamma_0_tau_tau`	Region 2, partial derivative, $\gamma^0_{\tau\tau}$	Table 13 of [1]
`R2_gamma_0_pi_tau`	Region 2, partial derivative, $\gamma^0_{\pi\tau}$	Table 13 of [1]
`R2_gamma_r_pi`	Region 2, partial derivative, γ^r_π	Table 14 of [1]
`R2_gamma_r_tau`	Region 2, partial derivative, γ^r_τ	Table 14 of [1]
`R2_gamma_r_pi_pi`	Region 2, partial derivative, $\gamma^r_{\pi\pi}$	Table 14 of [1]
`R2_gamma_r_tau_tau`	Region 2, partial derivative, $\gamma^r_{\tau\tau}$	Table 14 of [1]
`R2_gamma_r_pi_tau`	Region 2, partial derivative, $\gamma^r_{\pi\tau}$	Table 14 of [1]
`R2_specific_volume`	Region 2, specific volume, v	Table 12 of [1]
`R2_specific_int_energy`	Region 2, specific internal energy, e	Table 12 of [1]
`R2_specific_entropy`	Region 2, specific entropy, s	Table 12 of [1]
`R2_specific_enthalpy`	Region 2, specific enthalpy, h	Table 12 of [1]
`R2_cp`	Region 2, specific isobaric heat capacity, c_p	Table 12 of [1]
`R2_cv`	Region 2, specific isochoric heat capacity, c_v	Table 12 of [1]
`R2_sound_speed`	Region 2, specific of sound, w	Table 12 of [1]
`B2bc_p_from_h`	Region 2, boundary between 2b and 2c	Eqn. (20) of [1]
`B2bc_h_from_p`	Region 2, boundary between 2b and 2c	Eqn. (21) of [1]
`R2a_T_from_p_h`	Region 2a, backward function, $T = T(p, h)$	Eqn. (22) of [1]
`R2b_T_from_p_h`	Region 2b, backward function, $T = T(p, h)$	Eqn. (23) of [1]
`R2c_T_from_p_h`	Region 2c, backward function, $T = T(p, h)$	Eqn. (24) of [1]
`R2a_T_from_p_s`	Region 2a, backward function, $T = T(p, s)$	Eqn. (25) of [1]
`R2b_T_from_p_s`	Region 2b, backward function, $T = T(p, s)$	Eqn. (26) of [1]
`R2c_T_from_p_s`	Region 2c, backward function, $T = T(p, s)$	Eqn. (27) of [1]
`B23_p_from_T`	Region 2/3 boundary, p from T	Eqn. (5) of [1]
`B23_T_from_p`	Region 2/3 boundary, T from p	Eqn. (6) of [1]

Table 3: Supplementary equation for the metastable-vapor region implemented in IF97.h/C

Function Name	**Function Description**	**Reference**
`R2Meta_gamma_0`	Metastable-vapor region, dimensionless specific Gibbs free energy, ideal gas part, γ^0	Eqn. (16) of [1]
`R2Meta_gamma_r`	Metastable-vapor region, dimensionless specific Gibbs free energy, residual part, γ^r	Eqn. (19) of [1]
`R2Meta_gamma_0_pi`	Metastable-vapor region, partial derivative, γ^0_π	Table 13 of [1]
`R2Meta_gamma_0_tau`	Metastable-vapor region, partial derivative, γ^0_τ	Table 13 of [1]
`R2Meta_gamma_0_pi_pi`	Metastable-vapor region, partial derivative, $\gamma^0_{\pi\pi}$	Table 13 of [1]
`R2Meta_gamma_0_tau_tau`	Metastable-vapor region, partial derivative, $\gamma^0_{\tau\tau}$	Table 13 of [1]
`R2Meta_gamma_0_pi_tau`	Metastable-vapor region, partial derivative, $\gamma^0_{\pi\tau}$	Table 13 of [1]
`R2Meta_gamma_r_pi`	Metastable-vapor region, partial derivative, γ^r_π	Table 17 of [1]
`R2Meta_gamma_r_tau`	Metastable-vapor region, partial derivative, γ^r_τ	Table 17 of [1]
`R2Meta_gamma_r_pi_pi`	Metastable-vapor region, partial derivative, $\gamma^r_{\pi\pi}$	Table 17 of [1]
`R2Meta_gamma_r_tau_tau`	Metastable-vapor region, partial derivative, $\gamma^r_{\tau\tau}$	Table 17 of [1]
`R2Meta_gamma_r_pi_tau`	Metastable-vapor region, partial derivative, $\gamma^r_{\pi\tau}$	Table 17 of [1]
`R2Meta_specific_volume`	Metastable-vapor region, specific volume, v	Table 12 of [1]
`R2Meta_specific_int_energy`	Metastable-vapor region, specific internal energy, e	Table 12 of [1]
`R2Meta_specific_entropy`	Metastable-vapor region, specific entropy, s	Table 12 of [1]
`R2Meta_specific_enthalpy`	Metastable-vapor region, specific enthalpy, h	Table 12 of [1]
`R2Meta_cp`	Metastable-vapor region, specific isobaric heat capacity, c_p	Table 12 of [1]
`R2Meta_cv`	Metastable-vapor region, specific isochoric heat capacity, c_v	Table 12 of [1]
`R2Meta_sound_speed`	Metastable-vapor region, specific of sound, w	Table 12 of [1]

Table 4: Region 3 function implemented in IF97.h/C

Function Name	**Function Description**	**Reference**
`R3_phi`	Region 3, dimensionless specific Helmholtz free energy, ϕ	Eqn. (28) of [1]
`R3_phi_delta`	Region 3, partial derivative, ϕ_δ	Table 32 of [1]
`R3_phi_tau`	Region 3, partial derivative, ϕ_τ	Table 32 of [1]
`R3_phi_delta_delta`	Region 3, partial derivative, $\phi_{\delta\delta}$	Table 32 of [1]
`R3_phi_tau_tau`	Region 3, partial derivative, $\phi_{\tau\tau}$	Table 32 of [1]
`R3_phi_delta_tau`	Region 3, partial derivative, $\phi_{\delta\tau}$	Table 32 of [1]
`R3_p`	Region 3, pressure, p	Table 31 of [1]
`R3_specific_int_energy`	Region 3, specific internal energy, e	Table 31 of [1]
`R3_specific_entropy`	Region 3, specific entropy, s	Table 31 of [1]
`R3_specific_enthalpy`	Region 3, specific enthalpy, h	Table 31 of [1]
`R3_cp`	Region 3, specific isobaric heat capacity, c_p	Table 31 of [1]
`R3_cv`	Region 3, specific isochoric heat capacity, c_v	Table 31 of [1]
`R3_sound_speed`	Region 3, specific of sound, w	Table 31 of [1]

Table 5: Region 4 functions implemented in IF97.h/C

Function Name	Function Description	Reference
p_sat_from_T	Region 4, $p_{sat} = p_{sat}(T)$	Eqn. (30) of [1]
T_sat_from_p	Region 4, $T_{sat} = T_{sat}(p)$	Eqn. (31) of [1]

Table 6: Region 5 functions implemented in IF97.h/C

Function Name	Function Description	Reference
R5_gamma_0	Region 5, dimensionless specific Gibbs free energy, ideal gas part, γ^0	Eqn. (33) of [1]
R5_gamma_r	Region 5, dimensionless specific Gibbs free energy, residual part, γ^r	Eqn. (34) of [1]
R5_gamma_0_pi	Region 5, partial derivative, γ^0_π	Table 40 of [1]
R5_gamma_0_tau	Region 5, partial derivative, γ^0_τ	Table 40 of [1]
R5_gamma_0_pi_pi	Region 5, partial derivative, $\gamma^0_{\pi\pi}$	Table 40 of [1]
R5_gamma_0_tau_tau	Region 5, partial derivative, $\gamma^0_{\tau\tau}$	Table 40 of [1]
R5_gamma_0_pi_tau	Region 5, partial derivative, $\gamma^0_{\pi\tau}$	Table 40 of [1]
R5_gamma_r_pi	Region 5, partial derivative, γ^r_π	Table 41 of [1]
R5_gamma_r_tau	Region 5, partial derivative, γ^r_τ	Table 41 of [1]
R5_gamma_r_pi_pi	Region 5, partial derivative, $\gamma^r_{\pi\pi}$	Table 41 of [1]
R5_gamma_r_tau_tau	Region 5, partial derivative, $\gamma^r_{\tau\tau}$	Table 41 of [1]
R5_gamma_r_pi_tau	Region 5, partial derivative, $\gamma^r_{\pi\tau}$	Table 41 of [1]
R5_specific_volume	Region 5, specific volume, v	Table 39 of [1]
R5_specific_int_energy	Region 5, specific internal energy, e	Table 39 of [1]
R5_specific_entropy	Region 5, specific entropy, s	Table 39 of [1]
R5_specific_enthalpy	Region 5, specific enthalpy, h	Table 39 of [1]
R5_cp	Region 5, specific isobaric heat capacity, c_p	Table 39 of [1]
R5_cv	Region 5, specific isochoric heat capacity, c_v	Table 39 of [1]
R5_sound_speed	Region 5, specific of sound, w	Table 39 of [1]

Table 7: Helper functions implemented in IF97_helper.h/C

Function Name	Function Description	Reference
`findRegion`	Find region from (p, T)	Figure 1 of [1]
`genR3_sat_line`	To generate the saturation line properties in the section enclosed in Region 3, i.e., [623.15K, $T_{critical}$]	-
`genR4_sat_line`	To generate the saturation line properties in the section separating Region 1 and 2, i.e., [273.15K, 623.15K]	-
`R3_rho_from_p_T_ITER`	Region 3, $\rho = \rho(p, T)$, iterative method	-
`R3_T_x_from_p_h_ITER`	Region 3, T and x from (p, h), iterative method	-
`R3_T_x_from_p_s_ITER`	Region 3, T and x from (p, s), iterative method	-
`R3_dp_ddelta`	Region 3, partial derivative, $\left.\frac{\partial p}{\partial \delta}\right\|_{\tau}$	-
`R1_drho_dp`	Region 1, partial derivative, $\left.\frac{\partial \rho}{\partial p}\right\|_{T}$	-
`R2_drho_dp`	Region 2, partial derivative, $\left.\frac{\partial \rho}{\partial p}\right\|_{T}$	-
`R5_T_from_p_h_ITER`	Region 5, T from (p, h), iterative method	-
`R5_T_from_p_s_ITER`	Region 5, T from (p, s), iterative method	-

Table 8: Surface tension function implemented in SurfaceTension.h/C

Function Name	Function Description	Reference
`surf_tension`	Surface tension by saturation temperature, $\sigma = \sigma(T)$	The equation in [2]

Table 9: Viscosity function implemented in Viscosity.h/C

Function Name	Function Description	Reference
`mu0_bar`	Viscosity in the dilute-gas limit, $\bar{\mu}_0(\bar{T})$	Eqn. (11) in [3]
`mu1_bar`	Contribution to viscosity due to finite density, $\bar{\mu}_1(r\bar{h}o, \bar{T})$	Eqn. (12) in [3]
`viscosity`	Viscosity without critical enhancement ($\bar{\mu}_2 = 1$), $\mu = \mu(\rho, T)$	Eqn. (10) in [3]

Table 10: Thermal conductivity functions implemented in ThermalConductivity.h/C

Function Name	**Function Description**	**Reference**
`labmda0_bar`	Thermal conductivity in the dilute-gas limit, $\bar{\lambda}_0(\bar{T})$	Eqn. (16) in [4]
`labmda1_bar`	Contribution to thermal conductivity due to finite density, $\bar{\lambda}_1(r\bar{h}o, \bar{T})$	Eqn. (17) in [4]
`labmda2_bar`	Critical enhancement, $\bar{\lambda}_2(r\bar{h}o, \bar{T})$	Eqn. (18) in [4]
`zeta_R1`	$\zeta = \left(\frac{\partial \bar{\rho}}{\partial \bar{p}}\right)_{\bar{T}}$ in Region 1	Eqn. (24) in [4]
`zeta_R2`	$\zeta = \left(\frac{\partial \bar{\rho}}{\partial \bar{p}}\right)_{\bar{T}}$ in Region 2	Eqn. (24) in [4]
`zeta_R3`	$\zeta = \left(\frac{\partial \bar{\rho}}{\partial \bar{p}}\right)_{\bar{T}}$ in Region 3	Eqn. (24) in [4]
`zeta_REF`	$\zeta(\bar{\rho}, T_R)$	Eqn. (25) in [4]
`correlation_length_TC`	The correlation length, ξ	Eqn. (22) in [4]
`Zy`	Function Z(y)	Eqn. (21) in [4]
`thermal_conductivity _no_enhancement`	Thermal conductivity without critical enhancement ($\bar{\lambda}_2 = 0$)	Eqn. (15) in [4]
`thermal_conductivity_R1`	Thermal conductivity with critical enhancement, Region 1	Eqn. (15) in [4]
`thermal_conductivity_R2`	Thermal conductivity with critical enhancement, Region 2	Eqn. (15) in [4]
`thermal_conductivity_R3`	Thermal conductivity with critical enhancement, Region 3	Eqn. (15) in [4]

References

[1] "Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam", IAPWS R7-97, The International Association for the Properties of Water and Steam (IAPWS), August, 2007.

[2] "Revised Release on Surface Tension of Ordinary Water Substance", IAPWS R1-76, The International Association for the Properties of Water and Steam (IAPWS), June, 2014.

[3] "Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance", IAPWS R12-08, The International Association for the Properties of Water and Steam (IAPWS), September, 2008.

[4] "Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance", IAPWS R15-11, The International Association for the Properties of Water and Steam (IAPWS), September, 2011.