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

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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 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`	$\zeta(\bar{\rho}, \bar{T}_R)$	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.