Extrapolation of IAPWS Industrial Formulation IAPWS-IF97 to High Temperature above 800 °C

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The accuracies of IAPWS Industrial Formulation IAPWS-IF97 at high-temperature and high-pressure region out of its validity range have been tested. Although the behavior of IAPWS-IF97 is not very good for extrapolation, it still meets usual industrial requirements within some limited extrapolated region. IAPWS-IF97 equation for Region 2 can be extrapolated up to 30 MPa and 1300 K or 50 MPa and 1200 K with accuracies applied in the development of IAPWS-IF97.

Nomenclature

c_p	=	specific isobaric heat capacity
g	=	specific Gibbs free energy
h	=	specific enthalpy
T	=	thermodynamic temperature
p	=	Pressure
v	=	specific volume
w	=	speed of sound
z	=	any thermodynamic property
Δ	=	deviation from IAPWS-95

Subscripts

95	=	values calculated from IAPWS-95
97	=	values calculated from IAPWS-IF97
_2	=	IAPWS-IF97 Region 2 equation
_5	=	IAPWS-IF97 Region 5 equation
ref	=	reference deviation
max	=	maximum value

Introduction

In the long history of fossil fired steam power plant, its thermal efficiency has been mainly discussed from the viewpoint of economy, but it is now rather an environmental issue, because high efficiency is an important approach to reduce CO_2 emission. To meet today's environmental requirement, the main steam condition of power plant is quickly increasing. Temperatures above 900 K are being used in advanced power plants in Japan. In Europe, development of high temperature plant with 970 K has been started. Main steam pressures are also increasing up to 30 MPa or above.

In the near future, analysis of steam cycles with very high temperature above 1100 K, might be required in case studies. For such region, the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) [1] provides users with reliable information. It is valid up to 1273.15 K and can be extrapolated to higher temperatures.

However, engineers may want to extrapolate the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97)[2], whose upper limit temperature is 1073.15 K (800 °C) for the pressures above 10 MPa, because it is much faster than IAPWS-95 in computing speed and familiar in daily business. Information about the behavior of IAPWS-IF97 in the high-temperature region out of its validity range will be interesting for steam power engineers.

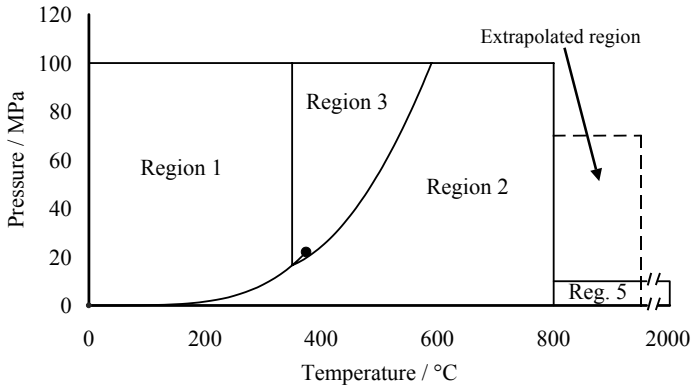

Fig. 1. Structure of IAPWS-IF97 and extrapolated region

Structure of IAPWS-IF97 and Extrapolations

Figure 1 shows the structure of IAPWS-IF97 on *p*-*T* plane. IAPWS-IF97 includes two $g(p,T)$ equations for super heated steam, namely equations for Region 2 and Region 5. An extrapolated region that is discussed in this paper is roughly shown by a quadrangle.

As seen, there are two possible extrapolations; the one is extrapolation of Region 2 equation to high-temperature side and the other is extrapolation of Region 5 equation to high-pressure side.

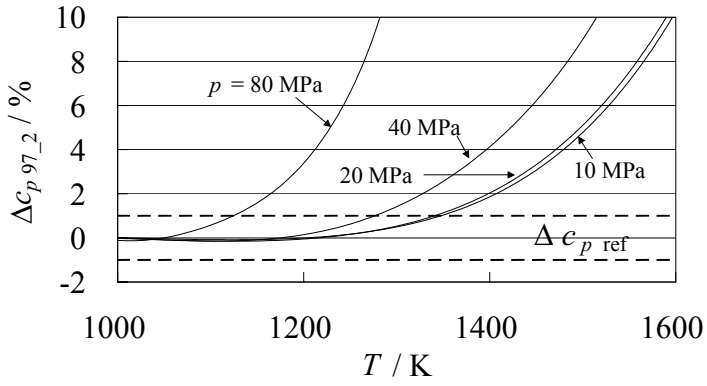

Fig. 2. Behavior of c_{p97_2}

Base of accuracy evaluation in the extrapolated region

IAPWS-IF97 equations have been fitted to IAPWS-95, and its accuracies have been evaluated by its deviation from the IAPWS-95. For *v* and *h*, the tolerances of the International Skeleton Tables IST-85[3] have been applied. For c_p and *w*, it has been specified that the deviations from IAPWS-95 should not exceed ±1 %.[4]

Industrial requirements on accuracy at the extrapolated region may vary dependent on the applications. In this paper, reference deviations were defined as follows.

For *v* and *h*, IST-85 does not specify the tolerance in the extrapolated region. For pressures from 10 to 80 MPa along the isotherm 1073.15 K, it is ±0.15 to ±0.3 % for *v* and ±8 to ±13 kJ kg^{-1} for *h*. In this paper, ±0.25 % and ±12 kJ kg^{-1} are used as the reference deviations Δv_{ref} and Δh_{ref} .

For c_p and *w*, ±1 % is used as $\Delta c_{p\mathrm{ref}}$ and Δw_{ref}.

Outlook on the behavior of IAPWS-IF97 equations in the extrapolated region

The IAPWS-IF97 equations are basically polynomials in the form of series of additions and multiplications. No exponential functions are used. It is a useful solution to achieve high computing speed[4]. It may, however, cause unfavorable behavior when the equations are extrapolated to outside of its validity range. Figure 2 shows sample plots of $\Delta c_{p97\_2} = (c_{p97\_2}-c_{p95})/c_{p95}$ along selected pressures. The deviation increases quickly in the high-temperature part of the extrapolated region and exceeds $\Delta c_{p\mathrm{ref}}$.

Figure 3 is similar but for Δc_{p97_5}. The deviation increases quickly in the high-pressure part of the extrapolated region.

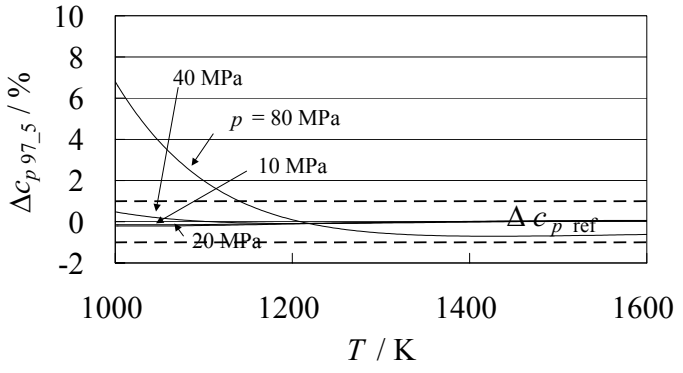

Fig. 3. Behavior of c_{p97_5}

Test of deviations from IAPWS-95

The deviations of IAPWS-IF97 from IAPWS-95 were tested in a range *p* = 0.5 to 70 MPa and *T* = 900 to 1600 K. The range was divided into 8 by 7 sections, 8 in the direction of *p* and 7 in the direction of *T*. The deviations Δz_{97} were evaluated at each section with 100,000 random input pairs of *p* and *T*.

Test results

Table 1 shows the maximum deviations of the IAPWS-IF97 equation.

Table 1. Maximum deviation of IAPWS-IF97 Region 2 equation in v, h, c_p, and w

	T = 900 to 1000 K	1000 to 1100 K	1100 to 1200 K	1200 to 1300 K	1300 to 1400 K	1400 to 1500 K	1500 to 1600 K
$\lvert\Delta v_{97\_2}\rvert_{max} = \lvert(v_{97\_2}-v_{95})/v_{95}\rvert_{max}$ /%							
p = 0.5 to 5 MPa	0.00	0.01	0.01	0.01	0.01	0.00	0.01
5 to 10 MPa	0.01	0.01	0.01	0.01	0.01	0.00	0.01
10 to 20 MPa	0.01	0.01	0.01	0.01	0.01	0.03	0.09
20 to 30 MPa	0.01	0.01	0.01	0.01	0.05	0.18	0.42
30 to 40 MPa	0.01	0.02	0.02	0.05	0.21	0.60	1.40
40 to 50 MPa	0.02	0.02	0.02	0.17	0.58	1.61	4.60
50 to 60 MPa	0.01	0.02	0.06	0.35	1.21	4.14	16.61
60 to 70 MPa	0.01	0.01	0.10	0.57	2.22	11.13	56.39
$\lvert\Delta h_{97\_2}\rvert_{max} = \lvert h_{97\_2}-h_{95}\rvert_{max}$ / kJ kg^{-1}							
p = 0.5 to 5 MPa	0.18	0.19	0.14	1.03	4.24	12.92	32.64
5 to 10 MPa	0.30	0.30	0.20	0.76	3.67	12.04	31.45
10 to 20 MPa	0.40	0.39	0.21	0.54	3.47	12.56	33.24
20 to 30 MPa	0.40	0.40	0.26	0.59	4.97	16.60	41.33
30 to 40 MPa	0.38	0.38	0.26	1.77	8.93	26.34	62.26
40 to 50 MPa	0.31	0.31	0.56	4.53	17.31	48.79	128.96
50 to 60 MPa	0.24	0.24	1.84	9.49	33.12	108.09	384.90
60 to 70 MPa	0.16	0.34	3.68	17.10	63.13	283.13	1264.70
$\lvert\Delta c_{p97\_2}\rvert_{max} = \lvert(c_{p97\_2}-c_{p95})/c_{p95}\rvert_{max}$ / %							
p = 0.5 to 5 MPa	0.09	0.04	0.14	0.67	2.05	4.98	10.47
5 to 10 MPa	0.10	0.08	0.08	0.56	1.92	4.82	10.30
10 to 20 MPa	0.09	0.14	0.15	0.53	2.03	5.10	10.71
20 to 30 MPa	0.10	0.17	0.17	0.79	2.68	6.23	12.37
30 to 40 MPa	0.11	0.17	0.17	1.41	4.11	8.97	17.82
40 to 50 MPa	0.11	0.14	0.53	2.61	7.06	17.05	44.38
50 to 60 MPa	0.10	0.13	1.22	4.64	13.56	47.09	171.11
60 to 70 MPa	0.07	0.36	2.20	7.87	30.01	155.43	587.41
$\lvert\Delta w_{97\_2}\rvert_{max} = \lvert(w_{97\_2}-w_{95})/w_{95}\rvert_{max}$ / %							
p = 0.5 to 5 MPa	0.02	0.02	0.02	0.07	0.22	0.50	0.97
5 to 10 MPa	0.03	0.02	0.01	0.06	0.20	0.50	1.02
10 to 20 MPa	0.03	0.04	0.05	0.05	0.31	0.80	1.56
20 to 30 MPa	0.04	0.07	0.07	0.22	0.80	1.82	3.36
30 to 40 MPa	0.04	0.07	0.13	0.74	2.05	4.42	8.72
40 to 50 MPa	0.04	0.06	0.45	1.75	4.49	10.45	23.23
50 to 60 MPa	0.06	0.11	0.92	3.18	8.53	22.16	42.35
60 to 70 MPa	0.09	0.17	1.34	4.68	14.56	35.17	61.78

for the region 2. The maximum deviations exceed the reference value Δz_{ref} at the grey-shaded sections in the table.

Specific heat capacity c_p is the strongest limiting factor for the extrapolation of the Region 2 equation. It limits the extrapolation to 30 MPa and 1300 K or 50 MPa and 1200 K.

Table 2 shows the test results for the Region 5 equation. Specific volume is the strongest limiting factor and it limits the extrapolation to 20 MPa. The pressure limit will not be attractive for modern steam power engineering.

Conclusions

Extrapolation of IAPWS-IF97 equations to high temperature region is possible with some extent. Users should carefully test if the accuracy of the equations in the extrapolated region meets their requirements. If the requirements are similar to those for IAPWS-IF97 development stage, Region 2 equation can be extrapolated up to 30 MPa and 1300 K or 50 MPa and 1200 K.

The extrapolation of Region 5 equation will not be attractive for modern steam power engineering.

Table 2. Maximum deviation of IAPWS-IF97 Region 5 equation in v, h, c_p, and w

	T = 900 to 1000 K	1000 to 1100 K	1100 to 1200 K	1200 to 1300 K	1300 to 1400 K	1400 to 1500 K	1500 to 1600 K
$\lvert\Delta v_{97\_5}\rvert_{max} = \lvert(v_{97\_5}-v_{95})/v_{95}\rvert_{max}$ / %							
p = 0.5 to 5 MPa	0.01	0.01	0.01	0.01	0.00	0.00	0.00
5 to 10 MPa	0.01	0.01	0.01	0.01	0.00	0.00	0.00
10 to 20 MPa	0.08	0.08	0.07	0.06	0.05	0.05	0.04
20 to 30 MPa	0.45	0.43	0.37	0.31	0.26	0.22	0.19
30 to 40 MPa	1.32	1.25	1.06	0.87	0.72	0.60	0.50
40 to 50 MPa	2.94	2.74	2.28	1.86	1.51	1.25	1.04
50 to 60 MPa	5.58	5.16	4.23	3.41	2.76	2.25	1.86
60 to 70 MPa	9.54	8.74	7.09	5.65	4.54	3.69	3.04
$\lvert\Delta h_{97\_5}\rvert_{max} = \lvert h_{97\_5}-h_{95}\rvert_{max}$ / kJ kg^{-1}							
p = 0.5 to 5 MPa	1.11	0.23	0.13	0.17	0.21	0.21	0.18
5 to 10 MPa	0.75	0.49	0.14	0.30	0.34	0.33	0.28
10 to 20 MPa	1.13	0.73	0.21	0.39	0.42	0.41	0.33
20 to 30 MPa	1.10	1.00	0.76	0.42	0.39	0.38	0.44
30 to 40 MPa	1.67	2.28	2.28	2.14	1.92	1.81	1.88
40 to 50 MPa	4.39	5.22	5.49	5.46	5.19	4.89	4.69
50 to 60 MPa	10.31	10.05	10.92	10.91	10.54	9.91	9.33
60 to 70 MPa	20.23	17.32	19.04	19.05	18.47	17.34	16.15
$\lvert\Delta c_{p97\_5}\rvert_{max} = \lvert(c_{p97\_5}-c_{p95})/c_{p95}\rvert_{max}$ / %							
p = 0.5 to 5 MPa	0.70	0.21	0.07	0.06	0.03	0.02	0.03
5 to 10 MPa	0.23	0.15	0.14	0.09	0.04	0.03	0.04
10 to 20 MPa	0.21	0.22	0.18	0.11	0.04	0.05	0.06
20 to 30 MPa	0.42	0.21	0.18	0.11	0.04	0.05	0.06
30 to 40 MPa	1.33	0.48	0.14	0.11	0.06	0.05	0.06
40 to 50 MPa	2.97	1.29	0.29	0.11	0.11	0.09	0.06
50 to 60 MPa	5.88	2.55	0.69	0.20	0.22	0.22	0.19
60 to 70 MPa	10.67	4.35	1.26	0.34	0.42	0.42	0.39
$\lvert\Delta w_{97\_5}\rvert_{max} = \lvert(w_{97\_5}-w_{95})/w_{95}\rvert_{max}$ / %							
p = 0.5 to 5 MPa	0.10	0.03	0.01	0.01	0.00	0.00	0.00
5 to 10 MPa	0.09	0.02	0.02	0.02	0.02	0.01	0.01
10 to 20 MPa	0.32	0.30	0.25	0.21	0.17	0.14	0.11
20 to 30 MPa	1.54	1.25	0.99	0.79	0.63	0.51	0.42
30 to 40 MPa	4.44	3.36	2.59	2.02	1.61	1.30	1.06
40 to 50 MPa	10.44	7.38	5.50	4.23	3.32	2.67	2.17
50 to 60 MPa	22.96	14.61	10.40	7.83	6.08	4.83	3.91
60 to 70 MPa	52.43	27.54	18.46	13.43	10.24	8.05	6.47

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References

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