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Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa

President:
Dr. Roberto Fernández-Prini
CNEA
Av. Libertador 8250
Buenos Aires-1429
Argentina

Executive Secretary:
Dr. R.B. Dooley
3412 Hillview Avenue
Electric Power Research Institute
Palo Alto, CA 94304-1395, USA

This release replaces the corresponding release of 1977 and contains 9 numbered pages.

This release has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its meeting in Erlangen, Germany, September 1997, for issue by its Secretariat. The members of IAPWS are Argentina, Canada, the Czech Republic, Denmark, Germany, France, Italy, Japan, Russia, the United Kingdom, and the United States of America.

Details about the equations presented in this release can be found in the article "A Formulation for the Static Permittivity of Water and Steam at Temperatures from 238 K to 873 K at Pressures up to 1200 MPa including Derivatives and Debye-Hückel Coefficients", by D.P. Fernández, A.R.H. Goodwin, E.W. Lemmon, J.M.H. Levelt Sengers, and R.C. Williams, published in the Journal of Physical and Chemical Reference Data **26**, 1125-1169 (1997) [1].

Further information about this release and other releases issued by IAPWS can be obtained from the Executive Secretary of IAPWS [2].

Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa

1. Nomenclature

g	Harris-Alder g-factor
k	Boltzmann's constant
M_w	Molar mass of water
N_A	Avogadro's number
p	pressure
T	absolute temperature, ITS-90
T_c	critical temperature
α	mean molecular polarizability of the isolated water molecule
ϵ	dielectric constant (relative permittivity)
ϵ_0	permittivity of free space
μ	dipole moment of the isolated water molecule
ρ	amount-of-substance (molar) density
ρ_c	critical density

2. Formulation

The Harris and Alder g-factor is given by

$$\frac{(\epsilon - 1)}{(\epsilon + 2)} = \frac{N_A \rho}{3}\left[\frac{\alpha}{\epsilon_0} + \frac{g\mu^2}{3kT\epsilon_0}\frac{9\epsilon}{(2\epsilon+1)(\epsilon+2)}\right] . \tag{1}$$

The values of the constants in this equation are given in Table 1.

Table 1. Constants used in the dielectric constant correlation [1]

Parameter	Value
Permittivity of free space, ϵ_0	$[4 \cdot 10^{-7}\ \pi\ (299\ 792\ 458)^2]^{-1}\ C^2 \cdot J^{-1} \cdot m^{-1}$
Mean molecular polarizability, α	$1.636 \cdot 10^{-40}\ C^2 \cdot J^{-1} \cdot m^2$
Molecular dipole moment, μ	$6.138 \cdot 10^{-30}$ C·m
Boltzmann's constant, k	$1.380\ 658 \cdot 10^{-23}\ J \cdot K^{-1}$
Avogadro's number, N_A	$6.022\ 136\ 7 \cdot 10^{23}\ mol^{-1}$
Molar mass of water, M_w	$0.018\ 015\ 268\ kg \cdot mol^{-1}$

Equation (1) is written as

$$\frac{\epsilon - 1}{\epsilon + 2} = A \frac{\epsilon}{(2\epsilon + 1)(\epsilon + 2)} + B \tag{2}$$

where A and B are given by

$$A = \frac{N_A \mu^2}{\epsilon_0 k} \frac{\rho g}{T} \tag{3}$$

$$B = \frac{N_A \alpha}{3\epsilon_0} \rho \tag{4}$$

The physically correct root of Eq. (2) for the dielectric constant is

$$\epsilon = \frac{1 + A + 5B + \sqrt{9 + 2A + 18B + A^2 + 10AB + 9B^2}}{4 - 4B} \tag{5}$$

Values of g can be determined from values of ϵ with the following equation:

$$g = (2 + \frac{1}{\epsilon}) \frac{kT}{3\mu^2} \left[\frac{3\epsilon_0}{N_A \rho} (\epsilon - 1) - \alpha(\epsilon + 2) \right] \tag{6}$$

The representation of g is

$$g = 1 + \sum_{h=1}^{11} N_h (\rho/\rho_c)^{i_h} (T_c/T)^{j_h} + N_{12} (\rho/\rho_c) \left(\frac{T}{228\ \mathrm{K}} - 1 \right)^{-1.2} \tag{7}$$

The values of N_h, i_h, and j_h are given in Table 2. The values of ρ_c and T_c, listed in Table 2, are those of the revised "Release on the Values of Temperature, Pressure and Density of Ordinary and Heavy Water Substances at their Respective Critical Points" (1992) [2].

Table 2. Coefficients N_h and exponents i_h and j_h of Eq. (7) for the g factor [1]

h	N_h	i_h	j_h
1	0.978 224 486 826	1	0.25
2	-0.957 771 379 375	1	1
3	0.237 511 794 148	1	2.5
4	0.714 692 244 396	2	1.5
5	-0.298 217 036 956	3	1.5
6	-0.108 863 472 196	3	2.5
7	$0.949\,327\,488\,264 \cdot 10^{-1}$	4	2
8	$-0.980\,469\,816\,509 \cdot 10^{-2}$	5	2
9	$0.165\,167\,634\,970 \cdot 10^{-4}$	6	5
10	$0.937\,359\,795\,772 \cdot 10^{-4}$	7	0.5
11	$-0.123\,179\,218\,720 \cdot 10^{-9}$	10	10
12	$0.196\,096\,504\,426 \cdot 10^{-2}$		

$\rho_c = 322/M_w\ \mathrm{mol \cdot m^{-3}}$ $\quad T_c = 647.096\ \mathrm{K}$

3. Equation of State of Water and Steam

In the conversion of the input independent variable pressure to density, preceding the optimization of Eq. (7), the "IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use" [3] has been used. In employing Eqs. (6, 7), with the constants in Tables 1, 2, for calculating the dielectric constant as a function of pressure, the IAPWS Formulation 1995 should be used.

4. Range of Validity of the Formulation

The formulation is valid in the range

from 238 to 273 K in the metastable liquid at atmospheric pressure (0.101 325 MPa);

from 273 to 323 K at pressures up to the lower of the ice VI melting pressure or 1000 MPa;

above 323 K at pressures up to 600 MPa.

The formulation extrapolates smoothly up to at least 1200 K and 1200 MPa.

5. Estimates of Uncertainty

Estimated absolute uncertainties in various regions of application are indicated in Table 3. Because of insufficient experimental data in most of the subregions, these estimates could not be based on rigorous statistics [1].

Table 3. Estimated absolute uncertainty U_ϵ of the predicted dielectric constant ϵ_{pred} at various state points

p/MPa	T/K	ρ/kg·m^{-3}	ϵ_{pred}	U_ϵ
0.101 325	*238*	*975.06*	*106.31*	*1*
0.101 325	*256*	*995.25*	*95.20*	*0.3*
0.101 325	*273*	*999.83*	*87.96*	*0.04*
585.3	273	1180	107.06	0.05
0.101 325	323	988.10	69.96	0.04
1230	323	1258	97.76	0.04
0.101 325	373	958.46	55.57	0.2
495.9	373	1110	67.73	0.5
3.1654	510	15.832	1.122	0.003
141.68	523	900	32.23	1
14.757	614	94.29	1.77	0.02
22.0385	647	358	6.19	0.3
19.9337	673	100	1.75	0.1
407.896	673	900	23.60	0.5
27.099	773	100	1.66	0.2
581.908	773	900	20.16	0.5
124.707	873	450	6.28	0.4

Values in italics are for metastable fluid states.

6. Values for Program Verification

In Table 4, dielectric constant values at selected entries of temperature and pressure are listed. The large number of digits is for the purpose of code verification; it does not reflect the uncertainty of the values.

Table 4. Density and dielectric constant values at given (p, T) state points

p/MPa	T/K	ρ/mol · dm^{-3}	ϵ
0.101 325	*240*	*54.337 01*	*104.349 82*
0.101 325	300	55.317 35	77.747 35
10	300	55.561 48	78.112 69
1000	*300*	*68.692 65*	*103.696 32*
10	650	2.246 92	1.267 15
100	650	40.310 90	17.717 33
500	650	52.586 36	26.621 32
10	870	1.452 75	1.127 21
100	870	20.989 27	4.982 81
500	870	45.013 76	15.097 46

Values in italics are for metastable fluid states.

7. References

[1] D.P. Fernández, A.R.H. Goodwin, E.W. Lemmon, J.M.H. Levelt Sengers, and R.C. Williams, J. Phys. Chem. Ref. Data, **26**, 1125-1169 (1997).

[2] IAPWS releases prepared up to 1994 have been published in Proc. 12th ICPWS, Orlando, FL, (1994), H.J. White, Jr., J.V. Sengers, D.B. Neumann, and J.C. Bellows (Eds.), Begell House, New York (1995). Up-to-date versions can be obtained from the Executive Secretary of IAPWS, Dr. R.B. Dooley, Electric Power Research Institute, 3412 Hillview Avenue, Palo Alto, CA 94304-1395, USA.

[3] Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use, Fredericia, Denmark, September 1996.