NOTES

New Equations for Computing Vapor Pressure and Enhancement Factor

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ABSTRACT

Equations are presented which relate saturation vapor pressure to temperature for moist air. The equations are designed to be easily implemented on a calculator or computer and can be used to convert in either direction. They are more accurate than the commonly used Goff-Gratch equations for the meteorologically interesting region of −80 to +50°C. Equations also are given for the enhancement factor.

1. Introduction

It frequently is necessary in meteorology and other related disciplines to calculate saturation vapor pressure from temperature, or vapor pressure from dewpoint temperature. These values are commonly obtained from the Goff-Gratch formulations (Goff and Gratch, 1946) as presented in the Smithsonian Tables (List, 1949) or from one of the many empirical equations which have appeared in the literature (e.g., Murray, 1967; Richards, 1971; Tabata, 1973; Lowe, 1977; Rasmussen, 1978), all of which use the Goff-Gratch formulation as a standard for comparison. A useful survey of those equations appears in Sargent (1980).

In the years since Goff and Gratch published their work, however, new and more accurate measurements were made of the vapor pressure of water from 25 to 100°C (Stimson, 1969) and at its triple point (Guildner *et al.*, 1976). In addition, new gas thermometry data made it possible to relate the International Practical Temperature Scale of 1968 to thermodynamic temperatures (Guildner and Edsinger, 1976), and a new value for the gas constant was adopted (Cohen and Tayler, 1973). In 1976, Arnold Wexler at the National Bureau of Standards published new vapor pressure formulations over water and ice based on these and other new developments and measurements (Wexler, 1976, 1977).

This note presents equations for vapor pressure which have been optimized with respect to these more accurate formulations by Wexler over the meteorologically interesting range −80 to +50°C. They have been designed to be easily implemented on a calculator or computer, yet to retain reasonably good accuracy over the range of interest. Unlike Goff-Gratch and some of the empirical equations, the equations given here can be used to convert in either direction.

Also presented are short equations for the enhancement factors for moist air, which have been fit to the most recent measurements available (Hyland, 1975) over the range of interest to meteorologists. The enhancement correction is used when calculating the vapor pressure of moist air as opposed to pure water vapor.

Curve-fitting and optimization tend to be rather subjective procedures, involving value judgments as to the desired range over which an equation is fit, the relative importance of regions within the range, and the tradeoff between error and equation complexity. I have computed more than one equation for each conversion, each with a different combination of temperature range and equation complexity.

In the concluding section a single set of equations is recommended for general use.

2. Definitions

Pure water vapor is said to be saturated when it can exist in stable thermodynamic equilibrium with a plane surface of pure water or ice. At the interface, the water vapor has the same temperature and pressure as the condensed phase. Water vapor over supercooled (below 0°C) water is, strictly speaking, not in stable equilibrium but rather in metastable equilibrium.

The pressure which pure water vapor has in a state of saturation, called "saturation pressure," is a function of temperature only and is denoted by e_w or e_i for saturation with respect to water or ice, respectively.

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Moist air is said to be saturated when it exists in a state of equilibrium similar to that described above for pure water vapor. We shall refer to the water vapor partial pressure of saturated moist air as e'_w or e'_i. It is a function of temperature and air pressure.

The enhancement factor is defined as the ratio of the saturation vapor pressure of moist air to that of pure water vapor, and so is given by

$$f_w = e'_w/e_w, f_i = e'_i/e_i\,. \tag{1}$$

The dew-point or frost-point temperature (T_d and T_f) of a parcel of moist air is defined as the temperature where, at constant pressure and mixing ratio, it is saturated with respect to water or ice, respectively.

Vapor pressure (e') is defined as the vapor pressure of moist air at ambient temperature, or saturation vapor pressure at its dew or frost point. The relationships among the above terms are given by the following, where T = ambient temperature:

$$\left.\begin{array}{ll} e'_w = e_w(T)f_w(\mathrm{T, P}) & \text{with respect to water} \\ e'_i = e_i(T)f_i(T, P) & \text{with respect to ice} \end{array}\right\}, \tag{2a}$$

$$\left.\begin{array}{ll} e' = e_w(T_d)f_w(T_d, P) & \text{with respect to water} \\ e' = e_i(T_f)f_i(T_f, P) & \text{with respect to ice} \end{array}\right\}. \tag{2b}$$

Units used in the following discussion are T (°C), e (mb) and P (mb).

3. Vapor pressure

Several equations are given for vapor pressure, optimized for different temperature regions. The equations take the following forms:

$$\left.\begin{array}{r} e_w \\ e_i \end{array}\right\} = a \exp\left(\frac{bT}{T+c}\right) \quad (e \text{ vs } T), \tag{3a}$$

$$T = \frac{cz}{b-z} \quad (T \text{ vs } e), \tag{3b}$$

and

$$\left.\begin{array}{r} e_w \\ e_i \end{array}\right\} = a \exp\left[\frac{(b-T/d)T}{T+c}\right] \quad (e \text{ vs } T), \tag{4a}$$

$$T = (d/2)[b - z - (b-z)^2 - 4cz/d^{1/2} \quad (T \text{ vs } e), \tag{4b}$$

where $z = \ln(e_w/a)$ or $\ln(e_i/a)$.

Eq. (3) is the well-known Magnus formula (Magnus, 1844), used by Tetens (1930) with different coefficients and converted to its present form by Murray (1967). This form was chosen because of its simplicity and because it allows one to easily convert between temperature and saturation vapor pressure in either direction. Eq. (4) is a modification of (3) by Bögel (1979) to produce a better fit at the expense of somewhat greater complexity. Like Eq. (3), this form also has the advantage of reversibility.

The values to which the present equations are optimized, and the standard against which they are compared are Wexler's most accurate formulations: Eq. (15) (Wexler, 1976) for vapor pressure over water and Eq. (54) (Wexler, 1977) for vapor pressure over ice. Wexler's formulations are given below:

$$\begin{aligned} e_w\,(\mathrm{Wex}) = 0.01 \exp[&-2991.2729\theta^{-2} \\ &- 6017.01280\theta^{-1} + 18.87643854 \\ &- 0.028354721\theta + 0.17838301 \times 10^{-4}\theta^2 \\ &- 0.84150417 \times 10^{-9}\theta^3 + 0.44412543 \times 10^{-12}\theta^4 \\ &+ 2.858487 \ln\theta], \end{aligned} \tag{5a}$$

$$\begin{aligned} e_i\,(\mathrm{Wex}) = 0.01 \exp[&-5865.3696\theta^{-1} \\ &+ 22.241033 + 0.013749042\theta \\ &- 0.34031775 \times 10^{-4}\theta^2 + 0.26967687 \times 10^{-7}\theta^3 \\ &+ 0.6918651 \ln\theta], \end{aligned} \tag{5b}$$

where θ is absolute temperature in K.

Wexler constrained both equations to yield the same values at the triple point (0.01°C). Some representative values are listed in Table 1. Wexler estimates the uncertainty of those values to be a few tens of parts per million (ppm) for Eq. (5a) and to increase from 16 ppm at 0°C to 3560 ppm at −80°C for Eq. (5b). Although Wexler does not discuss vapor pressure over supercooled water, Eq. (5a), having a rational thermodynamic basis, provides the best available estimate and so is used for water values below zero. Supercooled conditions are often encountered with cooled mirror hygrometers, in which the mirror surface can easily maintain a layer of water at −15°C for hours or days.

Rather than calculate least-squares fits to Wexler's formulations, a "minimax" fitting procedure was used in which the maximum error is minimized over the specified temperature interval. This procedure was then modified to allow variable error weighting over the interval, which forces a better fit near the region of most interest at the expense of larger error near the extremes of the interval.

The equation coefficients, the intervals used, and the resultant maximum errors are presented in Table 2. The error functions are plotted in Figs. 1 and 2 along with errors produced by the Goff-Gratch equations and the Tetens coefficients (Murray, 1967). For reference, the percent error corresponding to 0.01°C is also plotted. For completeness, equations e_{w5} and e_{w6} were included for the interval 0–100°C, even though that lies outside the meteorologically interesting region. They are shown in Table 2 but not plotted.

4. The enhancement factor

The present equations, Wexler's formulations, and the Goff-Gratch formulation all relate the saturation

TABLE 1. Reference values for vapor pressure (mb) and enhancement factors, from Wexler (1976 and 1977) and Hyland (1975).

	Pure water		Enhancement factor f			Moist air at 1000 mb	
T (°C)	e_w	e_i	1000 mb	500 mb	250 mb	e'_w	e'_i
−80		0.0005481		1.0041	1.002		
−70		0.0026189		1.0036	1.0018		
−60		0.010820	1.0064	1.0032	1.0016		0.01089
−50		0.039402	1.0058	1.0029	1.0014		0.03963
−40	0.19047*	0.12849	1.0052	1.0026	1.0013	0.19146	0.12915
−30	0.5106*	0.38024	1.0047	1.0024	1.0012	0.5130	0.38203
−20	1.2563*	1.0328	1.0044	1.0022	1.0012	1.2618	1.0373
−10	2.8657*	2.5992	1.0041	1.0022	1.0012	2.8774	2.6098
0	6.1121	6.1115	1.00395	1.00219	1.00132	6.1360	6.1360
10	12.279		1.00388	1.00229		12.327	
20	23.385		1.004	1.00251		23.479	
30	42.452		1.00426	1.00284		42.633	
40	73.813		1.00467	1.00323		74.157	
50	123.45		1.00519			124.09	

* Extrapolation of Eq. (5a).

vapor pressure of pure water to temperature; a slight correction must be made when one is dealing with moist air rather than pure water vapor. This correction, called the enhancement factor, is a weak function of temperature and pressure, amounting to ~1/2% at sea level.

Several equations of different complexity have been fit to the best available determinations of enhancement factor, those by Hyland (1975). Values found by Hyland are listed in Table 1. Hyland estimates his uncertainties at 1000 mb to increase from 0.01% at 50°C to 0.06% at −50°C. He does not assign errors below −50°C. I have assumed ice values for temperatures below 0°C, since the expected difference between water and ice values below zero is 0.01% or less (Greenspan, 1976).

As in the preceding section, a minimax curve fitting procedure was used, with variable weighting over the interval chosen. The following equation was fit:

$$f = 1 + A + P[B + C(T + D + EP)^2]. \qquad (6)$$

The resultant coefficients are given in Table 3 and the corresponding error functions are plotted in Fig. 3. The equation was fit over the temperature ranges shown in the figure. (Note: f_1 is optimized for pressures > 800 mb while f_2 can be used from sea level to 200 mb.)

5. Calculating vapor pressure and temperature in moist air

To determine vapor pressure in moist air, pure phase vapor pressure is multiplied by the enhancement factor according to Eq. (2).

To calculate temperature from vapor pressure when the dependence of enhancement on temperature is ignored (f_1, f_2 or f_3), Eqs. (3b) or (4b) are used and $e_w = e'_w/f_w$ or $e_i = e'_i/f_i$ is substituted. For

TABLE 2. Coefficients for calculating the vapor pressure in mb of pure water as a function of temperature in °C, optimized for several temperature intervals.

Curve	Equation	a	b	c	d	Temperature interval (°C)	Absolute value and (location) of maximum relative errors (% and °C)
e_{w1}	3	6.1121	17.502	240.97	—	−20, 50	0.20 (−20, +50)
e_{w2}	3	6.1121	17.368	238.88	—	0, 50	0.05 (50)
e_{w3}	3	6.1121	17.966	247.15	—	−40, 0	0.06 (−40)
e_{w4}	4	6.1121	18.729	257.87	227.3	−40, 50	0.23 (−40)
e_{w5}	3	6.1121	17.123	234.95	—	0, 100	0.15 (15, 65, 100)
e_{w6}	4	6.1121	18.564	255.57	254.4	0, 100	0.03 (29, 78, 100)
e_{wT}	3	6.1078	17.27	237.3	—		3.29 (−40)
e_{i1}	3	6.1115	22.542	273.48	—	−80, 0	0.14 (−80)
e_{i2}	3	6.1115	22.452	272.55	—	−50, 0	0.02 (−38, −11)
e_{i3}	4	6.1115	23.036	279.82	333.7	−80, 0	0.06 (−80)
e_{iT}	3	6.1078	21.87	265.5	—		10.7 (−80)

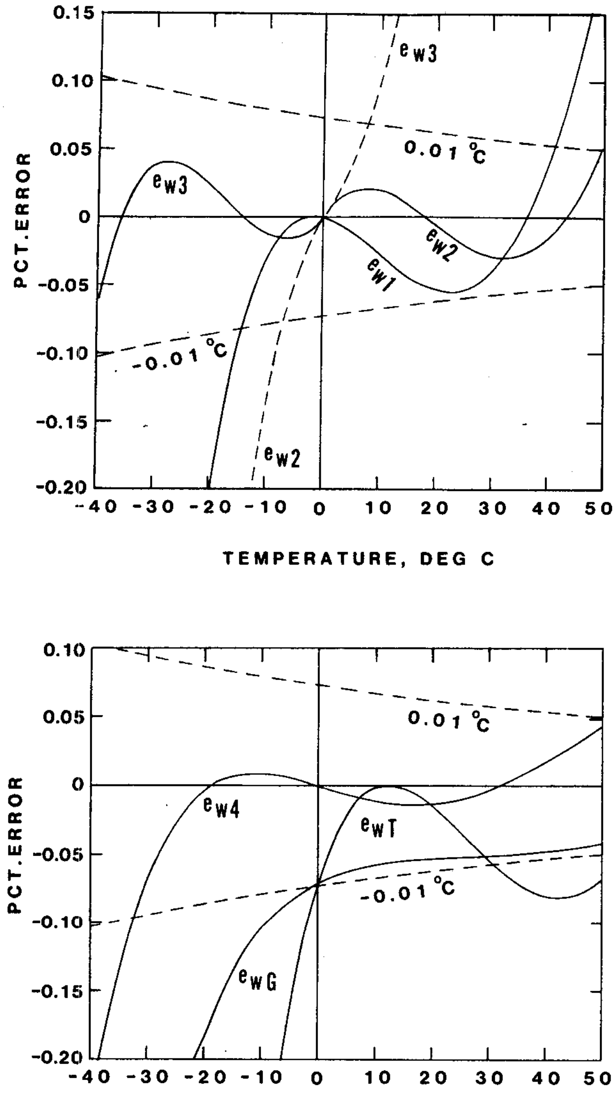

FIG. 1. Error functions for formulations of pure phase vapor pressure with respect to water. The curves give percent deviation from Wexler's values (Eq. 5a). Also included are error curves for the Goff-Gratch formulation (e_{wG}) and Tetens equation (e_{wT}) and curves corresponding to ±0.01°C temperature error.

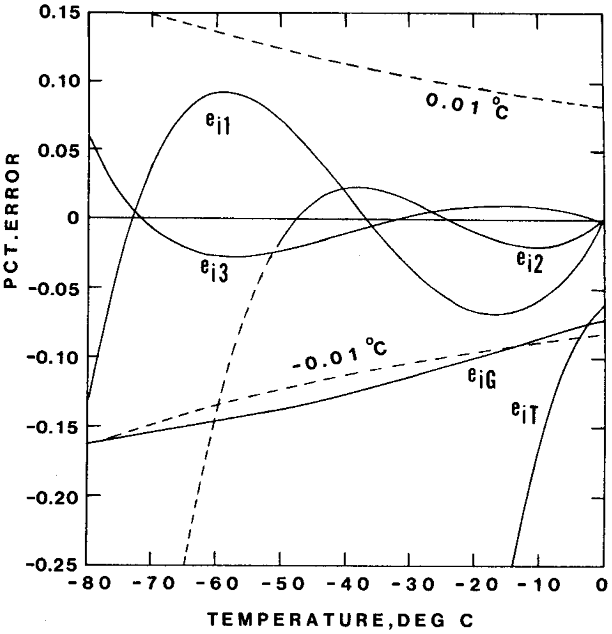

FIG. 2. Error functions for formulations of pure phase vapor pressure with respect to ice. The curves give percent deviation from Wexler's values (Eq. 5b). Also included are error curves for the Goff-Gratch formulations (e_{iG}) and Tetens equation (e_{iT}), and curves corresponding to ±0.01°C temperature error.

example, to calculate temperature T from saturation vapor pressure e'_w and P using curves e_{w1} and f_{w3}, we take the following steps:

$$T = 240.97z/(17.502 - z), \tag{7a}$$

where

$$z = \ln[e'_w/(6.1121 f_3)], \tag{7b}$$

and

$$f_3 = 1.0007 + 3.46 \times 10^{-6} P. \tag{7c}$$

When the temperature dependence of f is included, as in f_4 and f_5, a complication arises in calculating T from e because T is required in the calculation. However, since f is a very weak function of temperature, a rough approximation of T will serve nicely in calculating f.

TABLE 3. Coefficients for calculating the enhancement factor as a function of temperature in °C and pressure in mb, using Eq. (7).

Curve	A	B	C	D	E
f_{w1}, f_{i1}	4×10^{-3}	0	0	0	0
f_{w2}, f_{i2}	3.4×10^{-3}	0	0	0	0
f_{w3}	7×10^{-4}	3.46×10^{-6}	0	0	0
f_{i3}	3×10^{-4}	4.18×10^{-6}	0	0	0
f_{w4}	7.2×10^{-4}	3.20×10^{-6}	5.9×10^{-10}	0	0
f_{i4}	2.2×10^{-4}	3.83×10^{-6}	6.4×10^{-10}	0	0
f_{w5}	4.1×10^{-4}	3.48×10^{-6}	7.4×10^{-10}	30.6	-3.8×10^{-2}
f_{i5}	4.8×10^{-4}	3.47×10^{-6}	5.9×10^{-10}	23.8	-3.1×10^{-2}

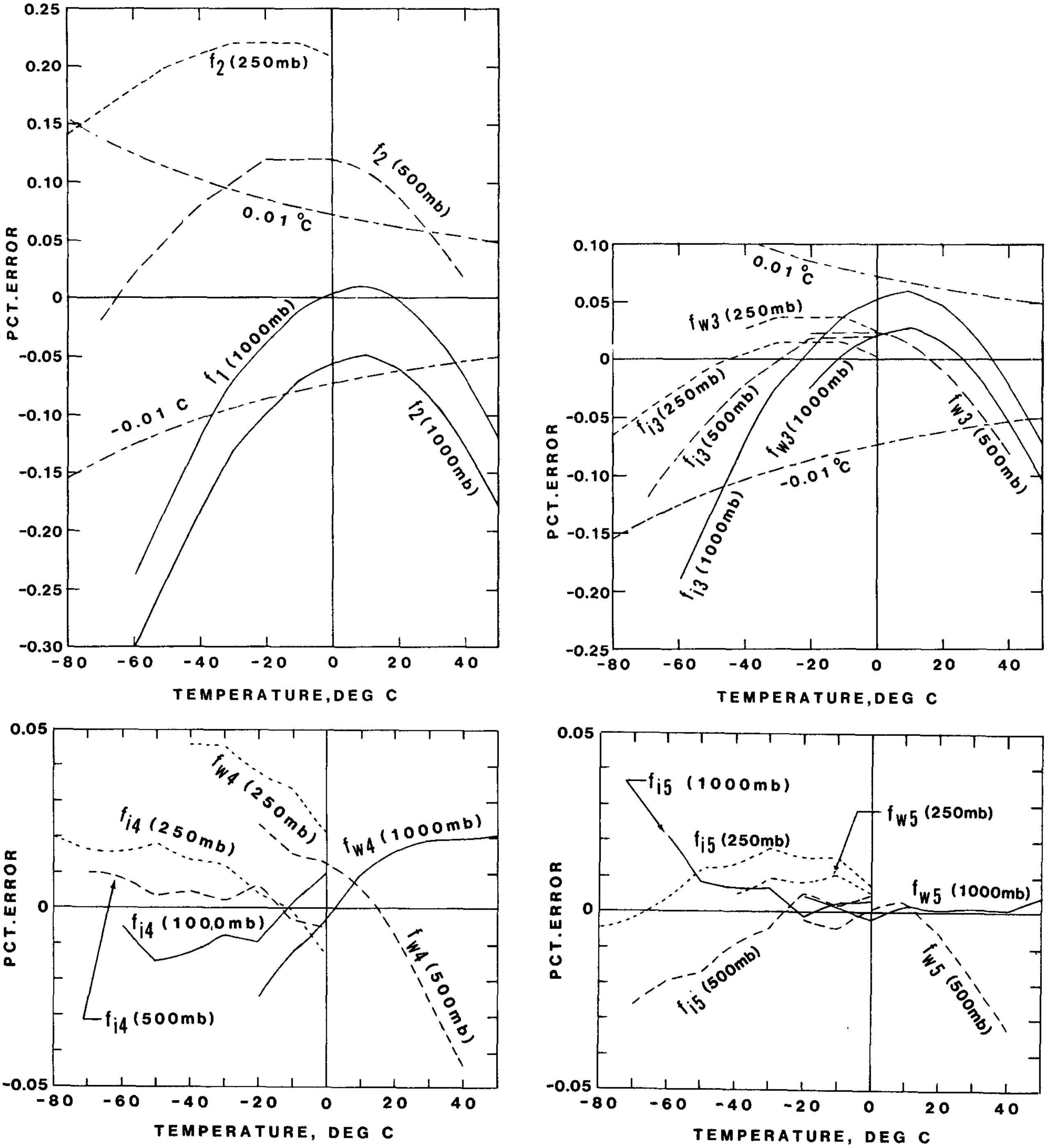

FIG. 3. Enhancement factor errors. The curves give percent deviation from Hyland's (1975) values. Curves corresponding to ±0.01 temperature error are also shown.

6. Discussion and recommendations

For some applications, these new equations will provide significant advantages over the older equations; for other applications there will be little improvement. It should be noted that experimental measurement errors are almost always larger than any of the errors found here, and that when an error term is much less than other contributing errors, further improvement in that term does not significantly improve overall error (see Revfeim, 1977, for further discussion).

In general, it is probably desirable to change to the new equations when significant error reduction is achieved in the range of interest, when computational speed is improved, or when it is desired to convert in both directions. Changing to the new equations is probably not justified when the error reduction is insignificant and/or when self-consistency is important in comparing new data with previously calculated data.

The degree of truncation for each coefficient was included in the optimizing computations to find the least number of significant places which could be used without significantly increasing the maximum error. Therefore, the coefficient values should not be further truncated.

For general use, curves e_{w1}, e_{i2}, f_{w3}, and f_{i3} are recommended. They are repeated here for convenience.

$$e'_w = [1.0007 + (3.46 \times 10^{-6} P)] \times 6.1121 \exp\left[\frac{17.502T}{240.97 + T}\right],$$

$$e'_i = [1.0003 + (4.18 \times 10^{-6} P)] \times 6.1115 \exp\left[\frac{22.452T}{272.55 + T}\right]. \quad (8)$$

Where computational simplicity is important, f_1 or f_2 should be used: f_1 in applications where pressure remains >800 mb, f_2 otherwise. When greater accuracy is desired, e_{w4}, e_{i3}, f_{w4} and f_{i4} are recommended. Other curves are appropriate for extreme conditions or special situations.

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