Polynomial Fits to Saturation Vapor Pressure

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ABSTRACT

The authors describe eighth- and sixth-order polynomial fits to Wexler's and Hyland–Wexler's saturation-vapor-pressure expressions. Fits are provided in both least-squares and relative-error norms. Error analysis is presented. The authors show that their method is faster in comparison with the reference expressions when implemented on a CRAY-YMP.

1. Introduction

We present eighth- and sixth-order polynomial fits to Wexler's (1976, 1977; hereafter named Wexler) and Hyland and Wexler's (1983; hereafter named Hyland–Wexler) saturation-vapor-pressure expressions (SVP) over water and ice. Also, fits to the temperature derivative of SVP are given. Very detailed comparison work has appeared recently (Gibbins 1990). Therefore, we do not review SVP formulations but proceed directly to develop numerical approximations suitable for use on modern computers. There are several reasons, related to numerical efficiency and accuracy of current approximations, for which we performed this work:

- Wexler's formulations are based on more recent experimental data than that of Goff and Gratch (1946) and Goff (1965) (hereafter named Goff–Gratch).
- Polynomials provide good global fits amenable to vectorized implementation on modern computers. For example, Gibbins (1990) compared about 60 of the existing algorithms for SVP and showed that the sixth-order polynomial fit was the fastest of them all.
- Polynomial fits provided previously by Lowe (1974) are given in the minmax norm and are not optimal for typical atmospheric science applications where relative accuracy is needed. Our polynomial fits exceed the accuracy of Lowe's fits.
- We provide eighth-order fits that are an order of magnitude more accurate in comparison to sixth-order polynomial fits.
- We extend the temperature range for which our fits are valid, thus making them more suitable for use in extreme temperature conditions. This should make the fits suitable for use in mesoscale and global models, particularly those used for cirrus cloud simulations.

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2. Reference expressions for SVP and temperature derivatives of SVP

a. Wexler formulation

The following formulas by Wexler form the basis of our polynomial fits. Wexler's formulations are based on more recent experimental data than that of Goff–Gratch. The international practical temperature scale (IPTS-68) is used. The results are based on newer measurements of the vapor pressure (Stimson 1969) and on highly accurate measurements of the vapor pressure of water at its triple point (Guildner et al. 1976).

SVP over water (Pa):

$$\ln(e_{w,\mathrm{sat}}) = \frac{g_0 + (g_1 + \langle g_2 + g_7 \ln(T) + \{g_3 + [g_4 + (g_5 + g_6 T)T]T\}T\rangle T)T}{T^2}. \tag{2.1}$$

Temperature derivative of SVP over water (mb K^{-1}):

$$\frac{de_{w,\mathrm{sat}}}{dT} = e_{w,\mathrm{sat}} \frac{(\langle g_7 + \{g_3 + [2g_4 + (3g_5 + 4g_6 T)T]T\}T\rangle T - g_1)T - 2g_0}{T^3}. \tag{2.2}$$

SVP over ice (Pa):

$$\ln(e_{i,\mathrm{sat}}) = \frac{k_0 + \{k_1 + k_5 \ln(T) + [k_2 + (k_3 + k_4 T)T]T\}T}{T}. \tag{2.3}$$

Temperature derivative of SVP over ice (mb K^{-1}):

$$\frac{de_{i,\mathrm{sat}}}{dT} = e_{i,\mathrm{sat}} \frac{\{k_5 + [k_2 + (2k_3 + 3k_4 T)T]T\}T - k_0}{T^2}. \tag{2.4}$$

Coefficients g and k are given in Table 1. Expressions for derivatives are not provided in the Wexler papers. We checked the derivatives with the numerical differentiation (Press and Teukolsky 1991) code, and the results were excellent. This provides confidence in the numerical behavior of (2.2) and (2.4).

b. Hyland–Wexler formulation

In 1983, Hyland and Wexler published revised values of the thermodynamic properties of water and moist air. These values were based in part on information that became available after Wexler's 1976 and 1977 papers. The new thermodynamic temperature scale (TTS) was used with significant changes to IPTS-68. It should be noted that the TTS scale is a very close approximation to the very recent temperature scale ITS-90 (Preston-Thomas 1990). Maximum differences between TTS and ITS-90 are about 4 mK. Since the formulation of SVP on the ITS-90 was not available to us, we decided to fit the Hyland and Wexler (1983) formulas. These expressions are valid in a more limited range of temperatures than the Wexler expressions. The Hyland–Wexler formulas are

$$\ln e_{w,\mathrm{sat}} = \sum_{i=-1}^{3} h_i T^i + h_4 \ln T, \qquad (2.5)$$

which is valid for $273.15 \leqslant T \leqslant 473.15$ K, and

$$\ln e_{i,\mathrm{sat}} = \sum_{i=0}^{5} m_i T^{i-1} + m_6 \ln T, \qquad (2.6)$$

which is valid over the range $173.16 \leqslant T \leqslant 273.16$ K. Coefficients h and m are given in Table 2.

3. Polynomial fits

a. Basic concepts

We present a fit of Wexler's expressions (2.1)–(2.4) with the polynomial

$$e_{\mathrm{sat}} = a_1 + a_2(T - T_0) + \cdots a_{n+1}(T - T_0)^n, \qquad (3.1)$$

where T_0 is a conversion between degrees Celsius and kelvins. It is $T_0 = 273.15$ for Wexler and Hyland–Wexler, and $T_0 = 273.16$ for Goff–Gratch. Double precision code was run on a 32-bit workstation. The fits are done with the weighted least-squares method (Morris 1990). Two sets of weights arise naturally. Constant weights provide a fit that minimizes absolute deviation with respect to the reference values; we call this version the absolute, or least-squares, norm. If the relative error is of importance, weights inversely proportional to the original data values are used; this is the relative-error norm. Polynomial fits were proposed before by Lowe (1974), who used the minmax norm and fitted the Goff and Gratch (1946) and Goff (1965) SVP expressions. The minmax (Chebyshev) norm is similar to the one we label here as the least-square norm. The minmax fit finds the approximation that minimizes the maximum absolute error. The absolute error is defined as

$$\mathrm{abs} = |e_{\mathrm{fit}} - e_{\mathrm{exact}}|, \qquad (3.2)$$

and the relative error is given by

$$\mathrm{rel} = 100 \frac{|e_{\mathrm{fit}} - e_{\mathrm{exact}}|}{e_{\mathrm{exact}}} (\%). \qquad (3.3)$$

TABLE 1. Coefficients of Wexler's (1976, 1977) expressions for saturation vapor pressure over water and ice.

SVP over water	SVP over ice
$g_0 = -0.29912729 \times 10^4$	$k_0 = -0.58653696 \times 10^4$
$g_1 = -0.60170128 \times 10^4$	$k_1 = 0.2224103300 \times 10^2$
$g_2 = 0.1887643854 \times 10^2$	$k_2 = 0.13749042 \times 10^{-1}$
$g_3 = -0.28354721 \times 10^{-1}$	$k_3 = -0.34031775 \times 10^{-4}$
$g_4 = 0.17838301 \times 10^{-4}$	$k_4 = 0.26967687 \times 10^{-7}$
$g_5 = -0.84150417 \times 10^{-9}$	$k_5 = 0.6918651 \times 10^0$
$g_6 = 0.44412543 \times 10^{-12}$	
$g_7 = 0.2858487 \times 10^1$	

TABLE 2. Coefficients of Hyland and Wexler's (1983) expressions for saturation vapor pressure over water and ice.

SVP over water	SVP over ice
$h_{-1} = -0.58002206 \times 10^4$	$m_0 = -0.56745359 \times 10^4$
$h_0 = 0.13914993 \times 10^1$	$m_1 = 0.63925247 \times 10^1$
$h_1 = -0.48640239 \times 10^{-1}$	$m_2 = -0.96778430 \times 10^{-1}$
$h_2 = 0.41764768 \times 10^{-4}$	$m_3 = 0.62215701 \times 10^{-6}$
$h_3 = -0.14452093 \times 10^{-7}$	$m_4 = 0.20747825 \times 10^{-8}$
$h_4 = 0.65459673 \times 10^0$	$m_5 = -0.94840240 \times 10^{-12}$
	$m_6 = 0.41635019 \times 10^1$

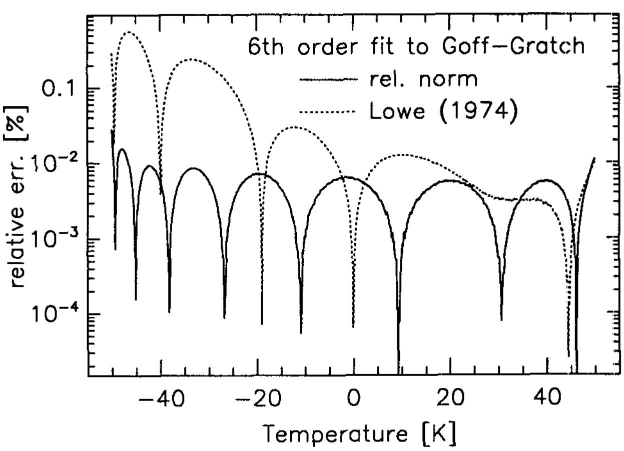

FIG. 1. Relative error for the sixth-order polynomial fit to the Goff–Gratch saturation vapor pressure over water for the temperature range −50°–50°C. Solid line is the fit performed with the relative norm. Dotted line presents Lowe's (1974) minmax norm results.

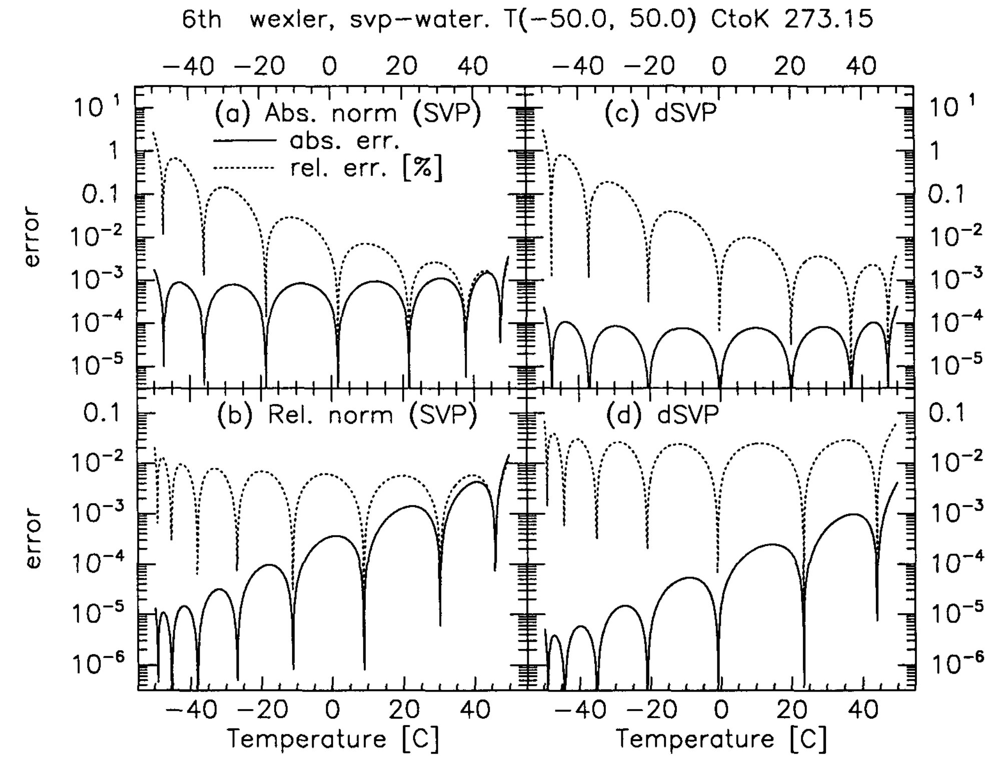

FIG. 2. Absolute (solid curves) and relative (dotted curves) errors for the sixth-order polynomial fit to the Wexler saturation vapor pressure and temperature derivative of saturation vapor pressure over water for the temperature range −50°–50°C. Results derived from applying both the absolute [(a) and (c)] and relative [(b) and (d)] norms are shown. Panels (a) and (b) are SVP, and (c) and (d) present temperature derivative of saturation vapor pressure.

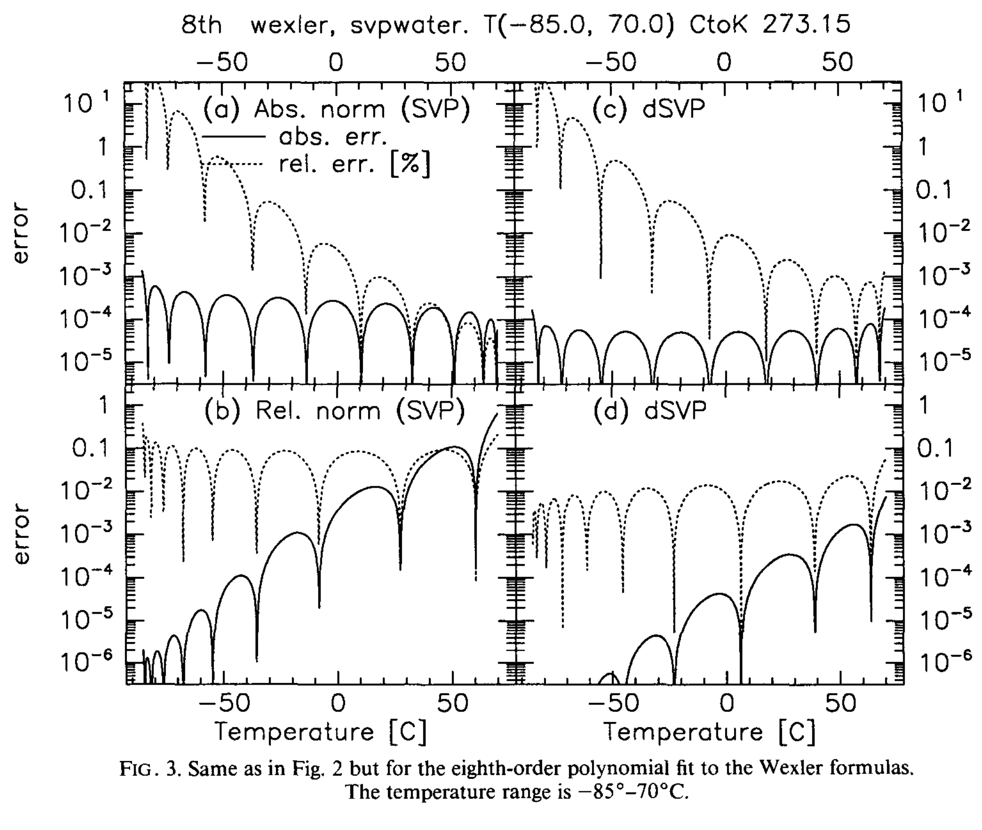

FIG. 3. Same as in Fig. 2 but for the eighth-order polynomial fit to the Wexler formulas. The temperature range is −85°–70°C.

In all of the figures that follow, the errors have positive values; the absolute value of errors is plotted. Figure 1 shows sixth-order polynomial fits to the Goff–Gratch formulas. The solid line shows results derived by us using the relative-error norm, and the dotted line is based on Lowe's (1974) sixth-order polynomial fit. It can be seen that our expressions are consistently better, with the exception of a small region of high temperatures. This, however, is the region where the error is already small. Thus, Lowe's fits are not optimal for the relative error. Use of the relative versus absolute norm is governed by the particular application. If a value of saturation vapor pressure is important in itself, the absolute-norm results should be used. On the other hand, if relative values are of importance (e.g., supersaturation), the relative-error norm is more natural.

b. Results

We present results of sixth- and eighth-order polynomial fits for SVP and its temperature derivative over water and ice. Plots of absolute and relative errors for SVP and the derivative of SVP over water are given in Figs. 2 and 3. In these figures, panels (a) and (b) present plots for SVP, and (c) and (d) for temperature derivative of SVP. All dashed lines show relative error in percent. All solid lines give absolute error. Panels (a) and (c) are for the absolute norm, while panels (b) and (d) are in the relative norm. The only difference between Figs. 2 and 3 is the order of polynomial (sixth and eighth, respectively) and the temperature range. Spikes on the plots correspond to the values where the polynomial "crosses" the reference data; that is, the predictions coincide. Notice that they are not distributed uniformly, with more spikes grouped in the low end of the temperature range. This is because low relative error for small values of saturation vapor pressure is difficult to achieve, and zeros of the polynomial have to be forced to satisfy the data exactly. When applying the relative norm (Figs. 2b, 3b, 2d, and 3d), the absolute error (solid line) increases with increasing temperature, but the relative error is fairly uniform if one ignores the spikes. Values of absolute or relative error equal to zero are removed because the data are plotted on a logarithmic scale. In contrast, application of the absolute norm (Figs. 2a, 3a, 2c, and 3c) causes the relative error (dotted line) to decrease sharply with increasing temperatures. It is very small at the high end of the temperature range. Absolute error remains fairly constant if one ignores the spikes. Table 3 gives the sixth-order Wexler fit in the temperature range −50°–50°C for water and −50°–0°C for ice. Table 4 gives the eighth-order Wexler fit in the temperature range −85°–70°C for water and −90°–0°C for ice. Table 5 gives the eighth-order Hyland–Wexler in the temperature range 0°–100°C for water and −75°–0°C for ice. The range −85°–70°C was chosen for application in a mesoscale model, where temperatures near −80°C may be encountered in the upper atmosphere (lower temperatures would be truncated to −85°C, which already has a near-zero SVP), and temperatures approaching 70°C might be encountered in desert soils, whose SVP must be evaluated.

TABLE 3. Coefficients of the sixth-order polynomial fits to SVP and its temperature derivative over water for the temperature range −50°–50°C. Same for ice but for the temperature range −50°–0°C. Results for the relative and absolute norms are given. The original data based on Wexler's formulation.

Coefficients	Relative error norm	Absolute norm
	Water vapor	Water vapor
a_1	6.11176750	6.11237757
a_2	0.443986062	0.443868373
a_3	0.143053301E-01	0.142972999E-01
a_4	0.265027242E-03	0.265277571E-03
a_5	0.302246994E-05	0.303440695E-05
a_6	0.203886313E-07	0.202923793E-07
a_7	0.638780966E-10	0.599234475E-10
	Ice	Ice
a_1	6.10952665	6.11129721
a_2	0.501948366	0.502946169
a_3	0.186288989E-01	0.187819100E-01
a_4	0.403488906E-03	0.413580047E-03
a_5	0.539797852E-05	0.572443200E-05
a_6	0.420713632E-07	0.471826455E-07
a_7	0.147271071E-09	0.178255421E-09
	Derivative; water	Derivative; water
a_1	0.444010270	0.443994807
a_2	0.286175435E-01	0.285899617E-01
a_3	0.795246610E-03	0.794469942E-03
a_4	0.120785253E-04	0.121487375E-04
a_5	0.101581498E-06	0.103456665E-06
a_6	0.384142063E-09	0.354662108E-09
a_7	0.669517837E-13	−0.690147330E-12
	Derivative; ice	Derivative; ice
a_1	0.503176636	0.503214671
a_2	0.376859982E-01	0.377082927E-01
a_3	0.126121755E-02	0.126471345E-02
a_4	0.244143919E-04	0.246483786E-04
a_5	0.291045085E-06	0.298694887E-06
a_6	0.203326382E-08	0.215398512E-08
a_7	0.647087051E-11	0.720715829E-11

4. Computer efficiency issues

Figure 4 presents the ratio of CRAY-YMP central processor time for three different saturation-vapor-pressure formulations. The upper figure compares Wexler's SVP over water to the eighth-order polynomial fit. The lower figure compares the Wexler and Magnus expressions. The abscissa indicates the length of the Fortran vector array containing temperatures used in the calculation. The eighth-order polynomial

TABLE 4. Coefficients of the eighth-order polynomial fits to SVP and its temperature derivative over water for the temperature range −85°–70°C. Same for ice but for the temperature range −90°–0°C. Results for the relative and absolute norms are given. The original data based on Wexler's formulation.

Coefficients	Relative error norm	Absolute norm
	Water vapor	Water vapor
a_1	6.11583699	6.11239921
a_2	0.444606896	0.443987641
a_3	0.143177157E-01	0.142986287E-01
a_4	0.264224321E-03	0.264847430E-03
a_5	0.299291081E-05	0.302950461E-05
a_6	0.203154182E-07	0.206739458E-07
a_7	0.702620698E-10	0.640689451E-10
a_8	0.379534310E-13	−0.952447341E-13
a_9	−0.321582393E-15	−0.976195544E-15
	Ice	Ice
a_1	6.09868993	6.11147274
a_2	0.499320233	0.503160820
a_3	0.184672631E-01	0.188439774E-01
a_4	0.402737184E-03	0.420895665E-03
a_5	0.565392987E-05	0.615021634E-05
a_6	0.521693933E-07	0.602588177E-07
a_7	0.307839583E-09	0.385852041E-09
a_8	0.105785160E-11	0.146898966E-11
a_9	0.161444444E-14	0.252751365E-14
	Derivative; water	Derivative; water
a_1	0.444035515	0.443956472
a_2	0.285991650E-01	0.285976452E-01
a_3	0.793972425E-03	0.794747212E-03
a_4	0.120923648E-04	0.121167162E-04
a_5	0.103673503E-06	0.103167413E-06
a_6	0.405898941E-09	0.385208005E-09
a_7	−0.579781423E-12	−0.604119582E-12
a_8	−0.115888324E-13	−0.792933209E-14
a_9	−0.318980675E-16	−0.599634321E-17
	Derivative; ice	Derivative; ice
a_1	0.503244909	0.503223089
a_2	0.377293671E-01	0.377174432E-01
a_3	0.126877355E-02	0.126710138E-02
a_4	0.250106092E-04	0.249065913E-04
a_5	0.316122722E-06	0.312668753E-06
a_6	0.262221927E-08	0.255653718E-08
a_7	0.139250559E-10	0.132073448E-10
a_8	0.432132775E-13	0.390204672E-13
a_9	0.598760960E-16	0.497275778E-16

fits are more efficient than the other formulations, running six times faster (in the asymptotic limit) than the accurate Wexler formulation.

5. Comments and conclusions

During the course of this study we investigated several approaches to numerical fits suitable for vector computers. There are some issues worth elaboration.

- Goff–Gratch: Replacement of the Goff–Gratch expressions (and numerous derivative formulations based on Goff–Gratch) in meteorological literature is long overdue. We present here Wexler and Hyland–Wexler formulations, but further improvements could be made by using the recently adopted ITS-90 scale.
- Uncertainties in the original data: There are uncertainties in the original data that are related to uncertainties in the measurements of temperature (temperature scales IPTS-68, TTS, ITS-90), triple point of

TABLE 5. Coefficients of the eighth-order polynomial fits to SVP and its temperature derivative over water for the temperature range 0°–100°C. Same for ice but for the temperature range −75°–0°C. Results for the relative and absolute norms are given. The original data based on Hyland–Wexler's formulation.

Coefficients	Relative error norm	Absolute norm
	Water vapor	Water vapor
a_1	6.11213476	6.11220713
a_2	0.444007856	0.443944344
a_3	0.143064234E-01	0.143195336E-01
a_4	0.264461437E-03	0.263350515E-03
a_5	0.305903558E-05	0.310636053E-05
a_6	0.196237241E-07	0.185218710E-07
a_7	0.892344772E-10	0.103440324E-09
a_8	−0.373208410E-12	−0.468258100E-12
a_9	0.209339997E-15	0.466533033E-15
	Ice	Ice
a_1	6.11123516	6.11153246
a_2	0.503109514	0.503261230
a_3	0.188369801E-01	0.188595709E-01
a_4	0.420547422E-03	0.422115970E-03
a_5	0.614396778E-05	0.620376691E-05
a_6	0.602780717E-07	0.616082536E-07
a_7	0.387940929E-09	0.405172828E-09
a_8	0.149436277E-11	0.161492905E-11
a_9	0.262655803E-14	0.297886454E-14
	Derivative; water	Derivative; water
a_1	0.444017302	0.444015587
a_2	0.286064092E-01	0.286078698E-01
a_3	0.794683137E-03	0.794390286E-03
a_4	0.121211669E-04	0.121452998E-04
a_5	0.103354611E-06	0.102353090E-06
a_6	0.404125005E-09	0.426886845E-09
a_7	−0.788037859E-12	−0.107509441E-11
a_8	−0.114596802E-13	−0.957713600E-14
a_9	0.381294516E-16	0.331271700E-16
	Derivative; ice	Derivative; ice
a_1	0.503277922	0.503265481
a_2	0.377289173E-01	0.377217899E-01
a_3	0.126801703E-02	0.126686507E-02
a_4	0.249468427E-04	0.248615257E-04
a_5	0.313703411E-06	0.310273831E-06
a_6	0.257180651E-08	0.249204696E-08
a_7	0.133268878E-10	0.122536732E-10
a_8	0.394116744E-13	0.316528423E-13
a_9	0.498070196E-16	0.264795683E-16

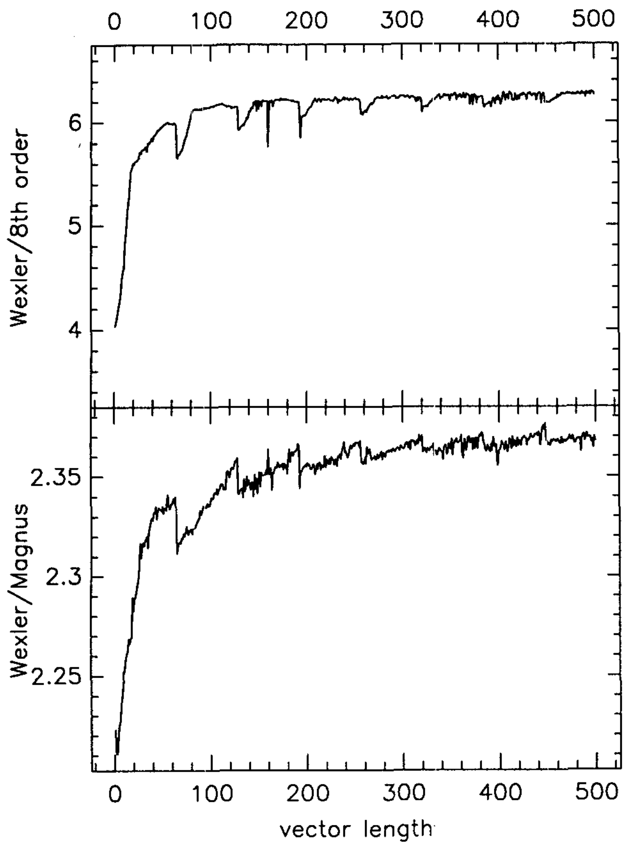

FIG. 4. Ratio of CRAY-YMP central processor time between three different saturation-vapor-pressure formulations. The upper figure compares Wexler's saturation vapor pressure over water to the eighth-order polynomial fit. The lower figure compares the Wexler expressions to Magnus (1844) expressions. The Magnus formula is used because it is one of the simplest expressions still retaining the exponential form. The abscissa indicates the number of elements of the Fortran vector (temperature) used in calculation.

water, and other experimental errors. This is described in more detail by Gibbins (1990). In this paper, we are as interested in computational technique as in the accuracy of vapor-pressure values, and have emphasized computational technique. For this reason we developed the Fortran code SVP, which can be used to generate fits of arbitrary order in specific temperature ranges and in user-defined SVP formulations. We also provide codes for Wexler, Hyland–Wexler, and Goff–Gratch formulations, but alternative formulations such as that of Haar et al. (1984) or SVP on the ITS-90 scale can be easily added. The code is available on request.

There is, however, reason to fit the data with accuracy exceeding that of an original measurement. Fits are often performed with functions of different analytical properties in comparison with the reference equation—fitting a polynomial to an exponential function is one example. Allowing for large errors in accuracy of a fit may result in very large errors of derived quantities such as; for example, the derivative.

- Rational approximations: Langlois (1967) presented fits to SVP in the form of a ratio of two polynomials P/Q. Such fits often exhibit excellent properties (Bender and Orszag 1978). Also, once one of the polynomials is calculated, it is "easier" to calculate the second one (because powers of independent variables can be precalculated). We performed such fits using the DIFCOR code (Kaufman et al. 1981). The results were excellent for the ratio of polynomials of sixth order. The more efficient eighth-order polynomial, however, provides sufficient accuracy.
- Economization of evaluation of polynomials: Knuth (1981) discusses algorithms that allow evaluation of the nth-order polynomials with fewer than n multiplications. Our test indicates that these algorithms lead to longer execution time on a CRAY because of memory reference and equivalence between addition and multiplication operations in chained calculations.
- Other approximations: Gibbins (1990) reviews more than 60 expressions for the approximation to SVP. Some of them are analytically more complex and numerically slower than the Goff–Gratch or Wexler expressions. We feel that unless applications clearly demand otherwise, the Wexler formulas should be used. Polynomial fits or table lookups could be considered for numerically intensive calculations.

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