On the Use of Finite Taylor's Series Approximations to Certain Exponential and Power Functions Employed in Cloud Models

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ABSTRACT

Poisson's equation for temperature and Murray's (1967) equation for saturation vapor pressure both can be replaced by an appropriate finite Taylor's series to produce computationally faster methods of solution. In the case of saturation vapor pressure, a Taylor's series of the standard Goff-Gratch equation results in increased accuracy as well as greater speed over Murray's formulation. It is suggested that other expressions commonly used in meteorological applications can be similarly replaced to allow both increased speed and possible gains in accuracy as well.

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1. Introduction

There are several mathematical expressions commonly found in meteorological applications having the form of an exponential or a power function. In terms of computer operations, such functions are rather time consuming because their complicated numerical algorithms require many additions, subtractions, divisions, and multiplications. (Raising to an integer power is roughly four times faster than raising to a non-integer power.)

This paper will demonstrate how a finite Taylor's series of an exponential or power function, for a modest investment of computer storage, may lead to a more expedient form involving a minimal number of multiplications and additions. Two frequently used functions will be considered: 1) saturation vapor pressure, an exponential function of temperature, and 2) Poisson's equation in which temperature is a power function of pressure. Since these functions must be evaluated repetitively at each finite time step and over a multitude of grid points in two- and three-dimensional models that include moist processes and the prediction of potential temperature, the saving in computer time when summed over the duration of a numerical experiment can be substantial. In the case of saturation vapor pressure, an added bonus of increased accuracy is achieved by developing a Taylor's series for the standard Goff-Gratch equation in lieu of the commonly used Tetens' equation (the magnus formula) as modified by Murray (1967) for computational expediency.

2. Saturation vapor pressure

Tabata's (1973) note on the calculation of saturation vapor pressure over liquid water prompted several responses in which accuracy and computational efficiency were the main issues. Hull (1974), [citing Murray, 1967], and Riegel (1974) each used a separate form of what is essentially Tetens' formula to indicate deficiencies in the accuracy and computational speed of Tabata's formulation. The accuracy of the Tetens equation, however, significantly degenerates with decreasing temperatures below 0°C. Wigley (1974) presented a method attributed to Richards (1971) that is highly accurate over a larger range of temperatures, yet is computationally inefficient for large numbers of calculations. An error analysis graphed by Wigley clearly shows that Richards' formula is by far the most accurate. Tetens' formula, vis-a-vis Murray's modification thereof, is next best in accuracy followed by the least accurate Tabata formula. Timing tests, to be discussed in greater detail later, show that Richards' method is about 40% slower than Murray's form of Tetens' equation. Although the Tabata formula was not actually timed, a straightforward estimate indicates that it is somewhat slower as well as less accurate than Murray's formula. Because of its relative efficiency and generally acceptable accuracy in the warmer temperature ranges, it is apparent why Murray's formula has become the most widely used of all saturation vapor pressure formulas. If a higher degree of accuracy is desired in the colder temperature ranges and speed is a crucial factor, it appears that one has to compromise accuracy or accept a loss in efficiency. This paper offers an alternative.

The respective methods of Murray, Richards, and Tabata, the latter with a change of logarithmic base, have the identical exponential form

$$e_s(T) = a_o \exp \{f(T)\} \tag{1}$$

in which each method is characterized by a unique constant a_o and temperature function $f(T)$. What distinguishes the individual methods in speed, though not necessarily in accuracy, is the complexity of $f(T)$. The highly accurate Richards formula also has the most complex $f(T)$, but Tabata's formula, though significantly less accurate than Murray's formula, has a slightly more complicated $f(T)$.

As stated in the introduction, exponentiation is an extremely slow computer operation. It is therefore proposed to replace (1) with a second order Taylor's series that yields a much faster algorithm with essentially the same accuracy as the original exponential form. Ogura (1963), in a shallow convection model, used a second order series of Tetens' equation to obtain a quadratic expression for potential temperature which was then used to establish a criterion for saturation, also noting the numerical convenience. The proposed Taylor's series is not limited to shallow convection and has several other advantages.

The series replacement of (1) has the form

$$e_s(T) = e_s(\overline{T})\{1 + T'[g(\overline{T}) + T'h(\overline{T})]\} \tag{2}$$

where

$$g(\overline{T}) = \frac{df(\overline{T})}{dT} \tag{3}$$

and

$$h(\overline{T}) = \tfrac{1}{2}\left\{\left[\frac{df(\overline{T})}{dT}\right]^2 + \frac{d^2f(\overline{T})}{dT^2}\right\} \tag{4}$$

in which $\overline{T}$ represents reference state temperatures and T' is the temperature deviation from the nearest reference state. The reference state saturation vapor pressures, $e_s(\overline{T})$, are precomputed using values of $\overline{T}$ in (1) and stored in a one-dimensional array. The values $e_s(\overline{T})$ are therefore as exact as the particular formula being transformed. The coefficients $g(\overline{T})$ and $h(\overline{T})$ are likewise precomputed and stored. Assuming a convergent series, it is obvious that (2) is increasingly in error from (1) as the absolute value of T' increases. In pursuit of rapid convergence of (2), with its minimal number of terms, $\overline{T}$ values are chosen to be integers such that T' always lies in the range $\pm \tfrac{1}{2}$ K. As will be shown, the integer $\overline{T}$ values conveniently serve as subscripts for the arrays corresponding to $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$.

The formulas of Richards and Murray both yield convergent series of the form given by (2). Tabata's formula was not considered because of its lack of accuracy. Since the coefficients of (2) are precomputed and stored, the transformed Richards and Murray equations are equal in computational speed as would be any formula transformable from (1) to (2). Naturally then, a logical choice is to use the transformed Richards formula to compute saturation vapor pressures since it provides excellent accuracy. Carrying this reasoning a step further, however, a convergent Taylor's series of the standard Goff-Gratch equation would result in a superior algorithm over any of the methods already discussed in terms of both speed and accuracy. The Goff-Gratch equation (List, 1958, p. 350) is not of the form (1) but is easily converted by a change of logarithmic base (Murray, 1967). The transformation to (2) then follows in a straightforward manner.

For saturation vapor pressure <u>over liquid water</u>, f(T) for the Goff-Gratch equation in form (1) follows directly from Murray (1967) as

$$f(T) = a_1 \frac{T_s}{T} + a_2 \ln \frac{T_s}{T} + a_3 \exp\left(a_4 \frac{T}{T_s}\right) + a_5 \exp\left(a_6 \frac{T_s}{T}\right) \qquad (5)$$

in which the included constants are

$a_o = 7.95357242 \times 10^{10}$, $a_1 = -18.1972839$, $a_2 = 5.02808$,
$a_3 = -70242.1852$, $a_4 = -26.1205253$, $a_5 = 58.0691913$,
$a_6 = -8.03945282$

and $T_s = 373.16$ K. The coefficients for (2), i.e., (3) and (4), are obtained by differentiating (5). The first and second derivatives of (5) which are needed for $g(\overline{T})$ and $h(\overline{T})$ are

$$\frac{df(T)}{dT} = -a_1 \frac{T_s}{T^2} - \frac{a_2}{T} + a_3 \frac{a_4}{T_s} \exp\left(a_4 \frac{T}{T_s}\right) - a_5 a_6 \frac{T_s}{T^2} \exp\left(a_6 \frac{T_s}{T}\right) \tag{6}$$

and

$$\frac{d^2 f(T)}{dT^2} = 2a_1 \frac{T_s}{T^3} + \frac{a_2}{T^2} + a_3\left(\frac{a_4}{T_s}\right)^2 \exp\left(a_4 \frac{T}{T_s}\right) + \left(a_5 a_6 \frac{T_s}{T^3}\right)\left(a_6 \frac{T_s}{T} + 2\right) \exp\left(a_6 \frac{T_s}{T}\right) \tag{7}$$

For saturation vapor pressure <u>over ice</u>, we again refer to Murray (1967). The Goff-Gratch equation in form (1) is thus characterized by

$$f(T) = a_1 \frac{T_o}{T} + a_2 \ln\left(\frac{T_o}{T}\right) + a_3\left(\frac{T}{T_o}\right) \tag{8}$$

with

$$a_o = 5.75185606 \times 10^{10}, \qquad a_1 = -20.947031$$

$$a_2 = -3.56654, \qquad a_3 = -2.01889049$$

and T_o = 273.16 K. Similarly to the case over liquid water, the Taylor's series coefficients for saturation vapor pressure over ice are obtained by differentiating (8). The required differentiation yields

$$\frac{df(T)}{dT} = -a_1 \frac{T_o}{T^2} - \frac{a_2}{T} + \frac{a_3}{T_o} \tag{9}$$

and

$$\frac{d^2 f(T)}{dT^2} = 2a_1 \frac{T_o}{T^3} + \frac{a_2}{T^2} \tag{10}$$

In summary, the series counterpart to the Goff-Gratch equation involves the precomputation and storage of reference state saturation vapor pressures, $e_s(\overline{T})$, and two corresponding coefficients, $g(\overline{T})$ and $h(\overline{T})$. Reference state e_s values are computed using (1) with the appropriate $f(T)$ for integer temperature values, $\overline{T}$. Reference state e_s values are exact. For saturation over liquid water, $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$ are precomputed with the aid of (5), (6), and (7). The appropriate equations for saturation over ice are (8), (9), and (10). The series method for calculating e_s is essentially embodied in (2) which, with its precomputed factors, provides an algorithm much faster than Murray's formula, yet is nearly as accurate as the exponential form of the Goff-Gratch formula.

The basic method of computing saturation vapor pressure using the series formulation proceeds in the following five steps:

1) Temperature, T, is computed or otherwise provided.

2) $\overline{T}$ is determined by rounding T to the nearest integer value.

3) T' is calculated as the difference $T - \overline{T}$. Note that $-\frac{1}{2}\ K \leq T' \leq \frac{1}{2}\ K$.

4) The subscript for the precomputed factors $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$ is calculated as the integer value $\overline{T}$ minus a reference value; e.g., if the scheme is set up for the temperature range 223 K to 323 K, the reference value for the subscript is 222. (In this way computer storage is minimized.)

5) Eq. (2) is now applied to determine the desired value of saturation vapor pressure.

The Appendix elucidates the method with a sample FORTRAN code. For the temperature range indicated in step 4, the factors $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$ require a modest 101 computer words each.

Since the series (2) is finite, a piecewise discontinuous representation of saturation vapor pressure results with discontinuities occurring at $\pm\ \frac{1}{2}$ K departures from integer temperature values. Fig. 1 shows the discontinuities for representative temperature intervals, emphasizing the slightness of the error. The accuracies of the methods of Richards,

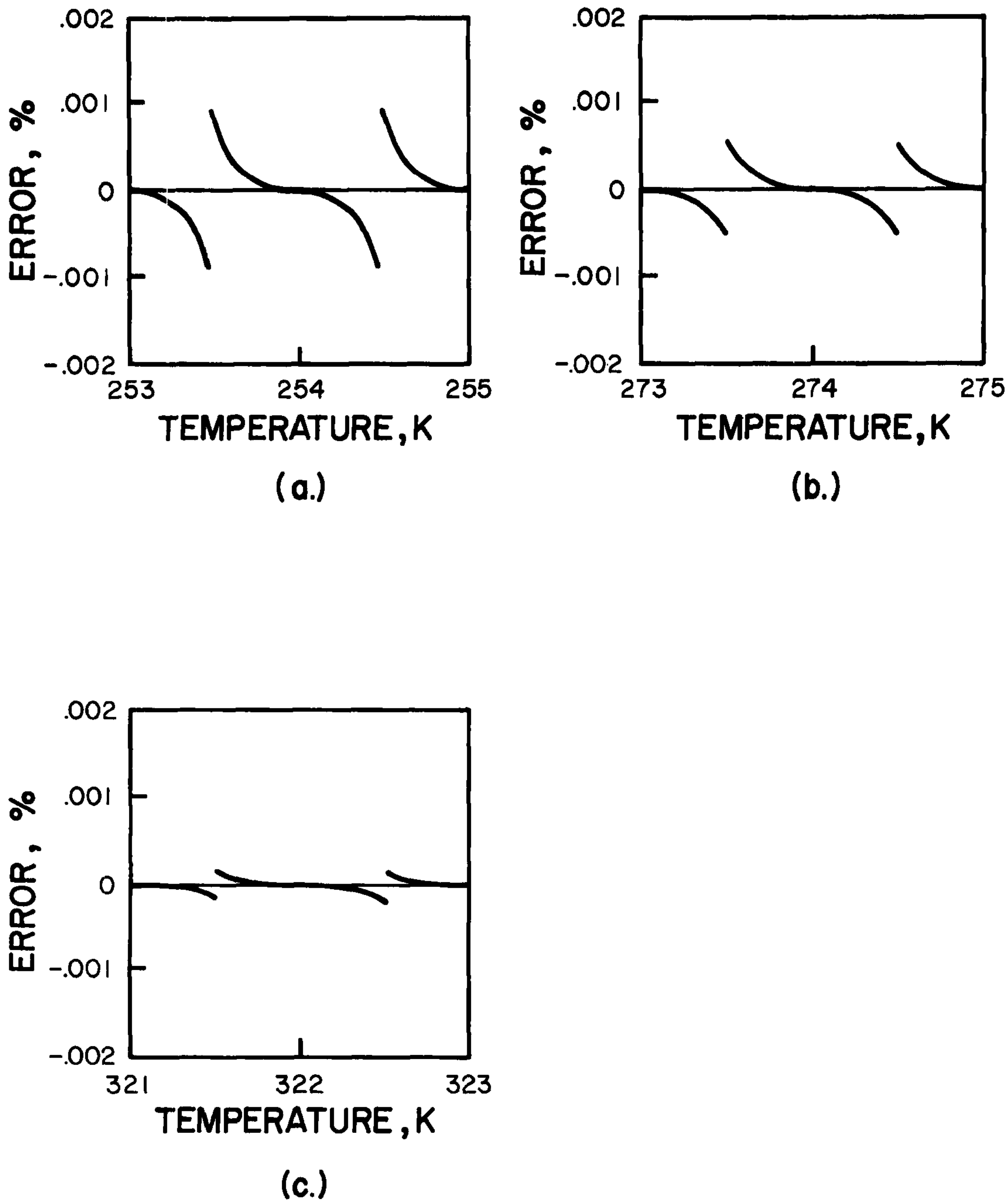

Fig. 1. Percentage error versus temperature for the second order Taylor's series of the Goff-Gratch equation, for the temperature ranges (a) 253-255 K, (b) 273-275 K, and (c) 321-323 K. Noting the vertical scale of the graphs, the discontinuities between integer temperature values are seen to be quite insignificant. This is for saturation vapor pressure over liquid water; the case over ice is comparable and is therefore not shown.

Tabata, and Murray appear in Fig. 2. The error of the series method, i.e., eq. (2), cannot be adequately plotted in Fig. 2 which has a vertical scale two orders of magnitude greater than Fig. 1. The series error would appear as a straight line along the zero error axis of Fig. 2. Looking at the figures, the superiority in accuracy of the Goff-Gratch series formulation becomes obvious.

Timing tests were made of the Goff-Gratch formulation, the series counterpart (including all 5 steps previously outlined), and the methods of Richards and Murray. Table 1 shows timing ratios of the various methods to the series method. Elapsed times are shown in Table 2, based on 10^7 calculations of e_s, which corresponds to a hypothetical 20 x 20 x 25 3-D model in which 10^3 time steps are taken. Timing tests were performed on four types of computer: a CDC-6400, a CDC-6600, a CDC-7600, and a Univac-1108. For each method of computing e_s, 5×10^3 calculations were completed and prorated to 10^7 calculations. Averaging the timing tests for the various computers, the series method is about 2.5 times faster than the commonly used Murray formulation.

The series method was then applied to a fully compressible 3-D moist convection model. With its acoustic disturbances, compressibility places a rigorous test on the series method. It was found that the discontinuities inherent in the method are indeed negligible and do not produce any trace of computational instability. Replacing (2), which is a second order series, with a third order series resulted in no discernible difference in the evolution of the model. A second order series of the Goff-Gratch equation is therefore quite appropriate. When compared to Murray's formulation, however, the series method produced an obviously different solution in the model that can be attributed only to the superior accuracy of the series method.

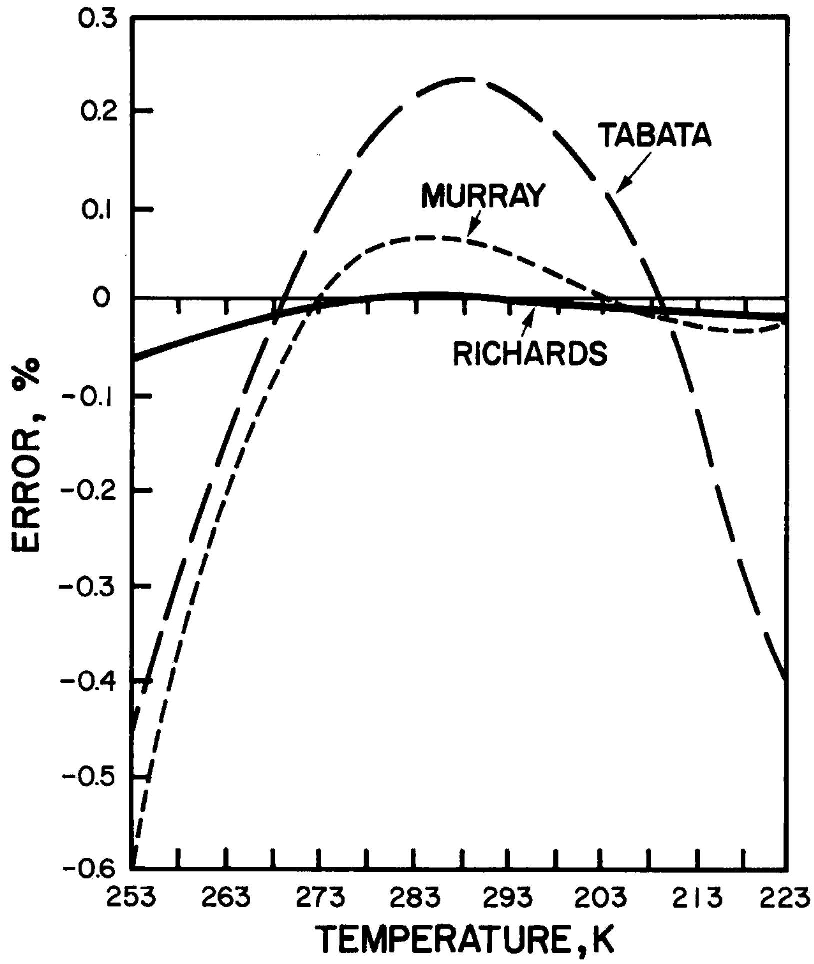

Fig. 2. Percentage error versus temperature for the formulas of Richards, Murray, and Tabata over liquid water. The analysis by Wigley (1974) was extended to emphasize the deterioration of Murray's values with decreasing temperatures. The Tabata error curve was taken directly from Wigley. The error curve of the Goff-Gratch series formulation would plot as a straight line along the zero axis for the given vertical scale.

Table 1. Ratios of the computational times of the various methods for computing saturation vapor pressure to the 2nd order Taylor's series of the Goff-Gratch formulation.

METHOD	CDC-6400	CDC-6600	CDC-7600	UNIVAC-1108
Goff-Gratch	10.58	8.18	9.31	9.33
2nd Order Series of Goff-Gratch	1.00	1.00	1.00	1.00
Murray (Tetens)	2.68	2.24	2.64	2.26
Richards	3.68	2.85	3.18	2.95

Table 2. Elapsed times of the various methods for computing saturation vapor pressure based on 10^7 calculations for each method. Time is in seconds.

METHOD	CDC-6400	CDC-6600	CDC-7600	UNIVAC-1108
Goff-Gratch	4883.1	1082.1	217.8	3500.9
2nd Order Series of Goff-Gratch	461.5	132.3	23.4	375.2
Murray (Tetens)	1236.7	296.5	61.9	851.1
Richards	1698.3	376.8	74.5	1109.2

When using the series method for computing saturation vapor pressure, one must be careful to develop the thermodynamics in a system of equations consistent with the accuracy of the Goff-Gratch equation. All expressions involving the temperature derivative of e_s, i.e., de_s/dT, should use the Clausius-Clapeyron equation, with no approximations, in which latent heat is a function of temperature. This offers no difficulty since latent heat can be represented quite acceptably as a linear function of temperature in the form

$$L = mT + b. \tag{11}$$

For the latent heat of vaporization, the constants b and m are equal to 3.150806×10^{10} and -2.379507×10^{7}, respectively, for units of ergs/gm.

3. Poisson's equation for temperature

Temperature, pressure, and potential temperature are related by the Poisson equation

$$T = \theta\left(\frac{P}{1000}\right)^{R/c_p} \tag{12}$$

A power function such as this is even slower to compute than an exponential due to its complex algorithm. Therefore, the factor $\left(\frac{P}{1000}\right)^{R/c_p}$, symbolized by π, is replaced by the second order Taylor's series

$$\pi = \pi_o\left\{1 + \frac{R}{c_p}\frac{P'}{P_o}\left[1 - \tfrac{1}{2}\frac{c_v}{c_p}\frac{P'}{P_o}\right]\right\} \tag{13}$$

in which $\pi_o = \left(\frac{P_o}{1000}\right)^{R/c_p}$, and P_o and P' are the pressure base state and deviation, respectively. The non-dimensional pressure, π_o, is a function of height only, and requires a one-dimensional array corresponding to the number of levels in a model. The constants $\frac{R}{c_p}$ and $\tfrac{1}{2}\frac{c_v}{c_p}$ are precalculated. The ratio $\frac{P'}{P_o}$, of course, is not calculated redundantly. With the use of (13), (12) is thus replaced by

$$T = \theta \pi_o \left\{ 1 + \frac{R}{c_p} \frac{P'}{P_o} \left[1 - \tfrac{1}{2} \frac{c_v}{c_p} \frac{P'}{P_o} \right] \right\} \tag{14}$$

A rigorous scale analysis by Dutton and Fichtl (1969) has shown that the ratio P'/P_o, i.e., the ratio of the pressure deviation to the reference state pressure at a given height, is quite small even in deep convection. Their analysis is substantiated by the computational results of Wilhelmson and Ogura (1972). Therefore, (14) should be quite valid for most applications. To test the validity of (14), a large P'/P_o was considered. The values θ = 305 K, P' = 3 mb, and P_o = 300 mb were employed, based on limiting values of P' observed in both numerical and field experimentation. This gives a value of .01 for P'/P_o.

For a complete analysis, a first order series of (12) was included along with (14). Relative accuracies are shown in Table 3. Comparisons of timing ratios and timing tests are given in Tables 4 and 5. On the average, (14) is about 5.0 times faster than (12), with a negligible deficit in accuracy.

As in the case of saturation vapor pressure, the Taylor's series counterpart to Poisson's equation was incorporated into a fully compressible 3-D model. A preliminary error analysis seemed to indicate that a second order series of (12) would be necessary for consistency in accuracy when employed in conjunction with the second order Goff-Gratch series formulation, (2). However, computational results showed no resolvable difference between using a first order or second order series of (12) despite the compressibility of the model. In fact, the only difference noted in comparing the use of a first order series versus the full Poisson equation was an obvious time saving. This lack of difference in the solution was due to the fact that the ratio P'/P_o remained much smaller than the extreme value .01 used to test (14). In general,

Table 3. Values of temperature computed by the various methods in which $\theta = 300$ K, $P_o = 300$ mb, and $P' = 3$ mb.

METHOD	TEMPERATURE COMPUTED, K
Poisson's Equation	216.84060
1st Order Series of Poisson's Equation	216.84279
2nd Order Series of Poisson's Equation	216.84058

Table 4. Ratios of the computational times of the various methods for computing temperature to the 2nd order series of Poisson's equation.

METHOD	CDC-6400	CDC-6600	CDC-7600	UNIVAC-1108
Poisson's Equation	5.24	4.96	5.45	4.26
1st Order Series of Poisson's Equation	0.67	0.80	0.43	0.72
2nd Order Series of Poisson's Equation	1.00	1.00	1.00	1.00

Table 5. Elapsed times of the various methods for computing temperature based on 10^7 calculations for each method. Time is in seconds.

METHOD	CDC-6400	CDC-6600	CDC-7600	UNIVAC-1108
Poisson's Equation	2567.7	601.9	102.4	1294.3
1st Order Series of Poisson's Equation	329.0	96.8	8.1	219.7
2nd Order Series of Poisson's Equation	490.3	121.3	18.8	303.9

a second order series of (12) should be used when combined with (2) unless there is a priori knowledge that P'/P_o will remain less than about .0075 in a numerical simulation.

4. Summary and conclusions

The benefits of using a Taylor's series approximation to the Goff-Gratch equation include superior accuracy and speed over other techniques for computing e_s. The discontinuities present in (2) were found to be quite negligible when the series method was applied to a compressible 3-D model. The requirement of additional computer storage for the precomputed factors $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$ is minimal, totaling 303 computer words for a 100 K temperature range. Therefore, the advantages of using a series formulation for e_s, especially in a large numerical model, far outweigh the single disadvantage of a slight cost in extra computer storage.

Similarly, replacing Poisson's equation, (12), with a first or second order Taylor's series yields a substantial gain in computational speed at the slight cost of storage for the precomputed factor π_o. The loss in accuracy by employing a second order series of (12) is negligible. A first order series introduces a slight error for a large value of P'/P_o. For consistency of accuracy, however, a second order series of (12) should be used in conjunction with using a second order series of the Goff-Gratch equation, unless P'/P_o in a simulation will always be less than .0075.

The combined use of the Taylor's series counterparts to the Goff-Gratch and Poisson equations resulted in a 5% time savings when applied to the comprehensive 3-D model. This is rather significant when considering that the calculation of temperature from pressure and potential temperature and the calculation of saturation vapor pressure constitute much less than 5% of the total number of required calculations in a comprehensive 3-D simulation.

In closing, it is suggested that of the many exponential and power functions appearing in meteorology, several would lend themselves to transformation into a finite Taylor's series to increase speed of computation. Even if many such modifications were incorporated into a numerical model, the cumulative need for increased computer storage for the precomputed factors appearing in the various series should not be prohibitive. In some cases such factors would be constant and not require arrays of memory. Finally, if a particular exponential or power function is an approximation to a more complicated expression, such as Murray's equation is approximate to the Goff-Gratch equation, a finite series of the more complicated expression could result in a gain in accuracy as well as speed over the approximate form.

APPENDIX

A sample FORTRAN code to describe the series method for computing saturation vapor pressure:

FORTRAN

```
1)  T  = ~~~
2)  IT  =  T + 0.5
3)  TDEL  =  T - IT
4)  L  =  IT - IREF
5)  EST  =  ES(L)* (1. + TDEL*(GT(L) + TDEL* HT(L)))
```

Explanation

1) T is computed.

2) T is rounded to nearest integer value.

3) T' is computed. Note that $-\frac{1}{2}$ K $\leq$ T' $\leq$ $\frac{1}{2}$ K.

4) Subscript for $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$ is determined from the integer temperature value; a reference value is subtracted to begin the subscripting at one.

5) Saturation vapor pressure is computed using T' and tabulated values of $e_s(\overline{T})$, $g(\overline{T})$, and $h(\overline{T})$.

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15. Supplementary Notes

16. Abstracts

Poisson's equation for temperature and Murray's (1967) equation for saturation vapor pressure both can be replaced by an appropriate finite Taylor's series to produce computationally faster methods of solution. In the case of saturation vapor pressure, a Taylor's series of the standard Goff-Gratch equation results in increased accuracy as well as greater speed over Murray's formulation. It is suggested that other expressions commonly found in meteorological applications can be similarly replaced for increased speed with possible gains in accuracy as well.

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Saturation vapor pressure
Application of finite Taylor's series to cloud models

17b. Identifiers/Open-Ended Terms

17c. COSATI Field/Group

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