SOME NOTES ON EXPONENTIAL ANALYSIS

By H. R. Grummann

Assistant Professor, Department of Applied Mathematics, Washington University

M. E. J. Geuhry de Bray in his charming little book "Exponentials made Easy"[1] tells how to determine the constants in the equation,

$$y = A_1\epsilon^{a_1x} + A_2\epsilon^{a_2x} \tag{I}$$

so that the curve will pass through four points, with equidistant ordinates on an empirical curve. If (Fig. 1) y_0, y_1, y_2, and y_3 are the equidistant ordinates and δ is their common separation, y_0 being the y intercept of the curve, de Bray's formulas are:

$$a_1 = \frac{\log z_1}{\delta}, \qquad a_2 = \frac{\log z_2}{\delta} \tag{II}$$

where z_1 and z_2 are the roots of the quadratic equation

$$\begin{vmatrix} z^2 & z & 1 \\ y_3 & y_2 & y_1 \\ y_2 & y_1 & y_0 \end{vmatrix} = 0. \tag{III}$$

The coefficients A_1 and A_2 of the two exponential terms are obtained by solving the two simultaneous equations

$$\begin{aligned} A_1 + A_2 &= y_0 \\ A_1 z_1 + A_2 z_2 &= y_1 \end{aligned} \tag{IV}$$

In attempting to find suitable empirical equations for some "river rating curves"—graphs of discharge versus stage—the writer tried to make use of de Bray's procedure. The original intention was to use the above method to determine the constants, and then to correct these constants by the use of Least Squares, as done by J. W. T. Walsh[2] in an application of the method to a problem in radioactivity. It often happens that a series of plotted observations suggest a simple exponential function, but that when the observations are replotted on semi-logarithmic paper a straight line is not obtained. Often, as in the case of a good many river rating curves, the result may be described

[1] Macmillan & Co. Ltd., St. Martin's St., London W. C. 2.

[2] Proceedings Phys. Soc. London XXXII. This reference is given by de Bray in his book, "Exponentials made Easy."

as "almost straight." At first blush it might seem that in all such cases it ought to be possible to fit a curve with equation I to the data by de Bray's Method. By an easy generalization of the above formulas, the constants in an equation with three or four exponential terms could be determined if two terms were not enough to secure a good fit.

It was soon found, however, that innocent looking monotonic curves without points of inflection plotted from data that gave an "almost straight" line on semi-logarithmic paper quite often led to a quadratic equation, (equation III) whose roots were not both positive numbers.

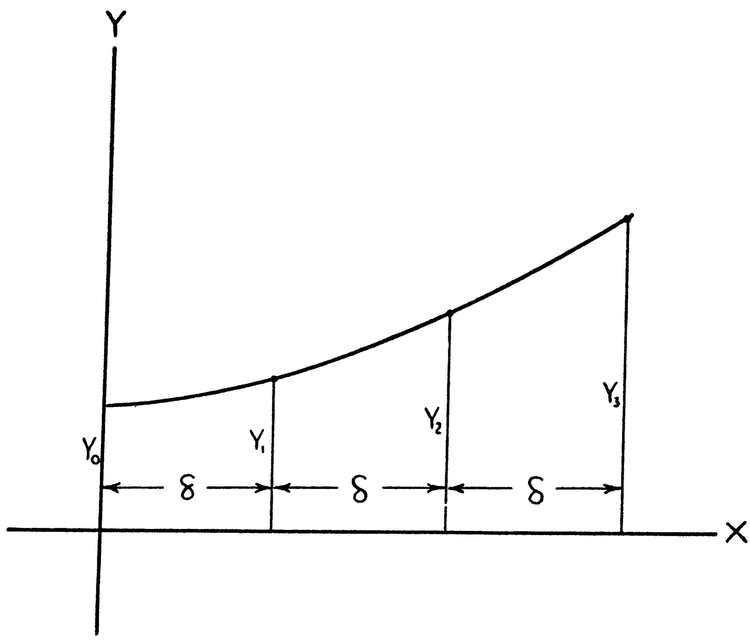

FIG. 1

If z_1 and z_2, the roots of III, are complex conjugates, it may be seen from IV that A_1 and A_2 will be complex conjugates. Also, a_1 and a_2 will be conjugate complex numbers and may be calculated as follows:

Let $z_1 = r\epsilon^{i\theta}$ and $z_2 = r\epsilon^{-i\theta}$
then from equation II,

$$r\epsilon^{i\theta} = \epsilon^{a_1\delta},$$

$$r\epsilon^{-i\theta} = \epsilon^{a_2\delta}$$

whence, by division to eliminate r we have

$$\epsilon^{2i\theta} = \epsilon^{\delta(a_1-a_2)}, \text{ or}$$

(Va) $$\frac{2i\theta}{\delta} = a_1 - a_2.$$

Also, by multiplication to eliminate θ,

$$r^2 = \epsilon^{\delta(a_1+a_2)}, \text{ or}$$

$$\text{(Vb)} \qquad \frac{2 \log r}{\delta} = a_1 + a_2.$$

The sum and difference of the two a's being obtained by these expressions, one may solve for a_1 and a_2.

Let $\quad a_1 = \lambda + \iota\mu \qquad A_1 = \alpha + \iota\beta$

$\quad a_2 = \lambda - \iota\mu \qquad A_2 = \alpha - \iota\beta$

Then equation I becomes

$$y = (\alpha + \iota\beta)\epsilon^{(\lambda+\iota\mu)x} + (\alpha - \iota\beta)\epsilon^{(\lambda-\iota\mu)x},$$

$$y = 2\epsilon^{\lambda x}[\alpha \cos \mu x - \beta \sin \mu x], \text{ or}$$

$$\text{(VI)} \qquad y = 2\epsilon^{\lambda x} R \cos (\mu x + c)$$

where $R = \sqrt{\alpha^2 + \beta^2}$ and $\tan c = \frac{\beta}{\alpha}$.

If one of the roots of III is negative, the de Bray formulas II and IV will still give an expression for equation I which formally reproduces y_0, y_1, y_2, and y_3 when 0, δ, 2δ, and 3δ, are substituted for x respectively, but which is useless for interpolating and of no value as a solution of the curve fitting problem. Suppose, for example, that z_1 is positive and z_2 is negative. Then

$$z_2 = (-1) \mid z_2 \mid \qquad \text{and}$$

$$\log z_2 = \log (-1) + \log \mid z_2 \mid .$$

Equation I then becomes

$$y = A_1\epsilon^{a_1x} + (-1)^{\frac{x}{\delta}} A_2\epsilon^{\frac{x \log |z_2|}{\delta}},$$

the factor $(-1)^{\frac{x}{\delta}}$ being real only when x is an integral multiple of δ. If the (-1) is written $e^{\iota\pi}$, we have

$$y = A_1\epsilon^{a_1x} + \epsilon^{\frac{\pi \iota x}{\delta}} A_2\epsilon^{\frac{x \log |z_2|}{\delta}}, \text{ or}$$

$$y = A_1\epsilon^{a_1x} + A_2\epsilon^{\frac{x \log |z_2|}{\delta}}\left[\cos \frac{\pi x}{\delta} + \iota \sin \frac{\pi x}{\delta}\right].$$

Neither the real nor the imaginary part would be a graduation function for a monotonic curve as each has a half period of δ.

The expression for I is similar, and of no greater practical value, if both of the roots of III are negative.

Without loss of generality we may let $y_0 = 1$, $r_1 = \frac{y_1}{y_0}$ $r_2 = \frac{y_2}{y_1}$ $r_3 = \frac{y_3}{y_2}$. Then the quadratic III becomes

$$\begin{vmatrix} z^2 & z & 1 \\ r_2 r_3 & r_2 & 1 \\ r_1 r_2 & r_1 & 1 \end{vmatrix} = 0, \qquad \text{or.}$$

written in the form

$$z^2 + pz + q = 0, \quad \text{i.e.,}$$

(IIIa)
$$z^2 + \frac{r_2(r_1 - r_3)}{(r_2 - r_1)} z + \frac{r_1 r_2 (r_3 - r_2)}{(r_2 - r_1)} = 0.$$

Hence the roots of this quadratic are real and unequal if $D > 6$, equal if $D = 6$, and complex if $D < 6$, where

$$D = \left[\frac{r_3}{r_1} - 3\frac{r_1}{r_3}\right] + 4\left[\frac{r_1}{r_2} + \frac{r_2}{r_3}\right]$$

From the point of view of the computer, however, it is about as much work to calculate D as to solve the quadratic equation.

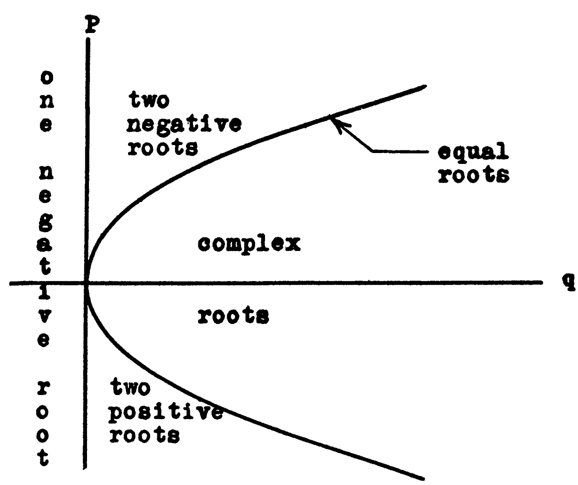

FIG. 2

Reverting to equation IIIa; suppose the numbers q and p are plotted as the coordinates of a point (q, p) as in Fig. 2. Then the parabola $p^2 = 4q$ is, so to speak, a locus of equal roots. The remainder of the figure requires no explanation.

Suppose that all the r's are positive, as they would be in the case of a simple monotonic curve which one proposed subjecting to an exponential analysis.

If $q < 0$, the quadratic will have one negative root. Now

$$q = \frac{r_1 r_2(r_3 - r_2)}{(r_2 - r_1)} \quad \text{and hence}$$

for $q < 0$, if $r_2 > r_1$, then $r_3 < r_2$ and consequently $r_3 < r_2 > r_1$ and if $r_2 < r_1$, then $r_3 > r_2$, or $r_1 > r_2 < r_3$. Also, provided $p_2 > 4q$, a positive p and a positive q will give two negative roots. But

$$p = \frac{r_2(r_1 - r_3)}{(r_2 - r_1)},$$

and p and q can not both be positive when all the r's are positive as this implies either that $r_2 > r_1$, $r_1 > r_3$ and $r_3 > r_2$, a contradiction, or else that $r_2 < r_1$, $r_1 < r_3$ and $r_3 < r_2$, also a contradiction. Hence if both roots are negative, the r's can not be all positive. The case of two negative roots will not arise in trying to fit equation I to a monotonic curve, since if all the r's are positive both p and q can not be positive.

For all r's positive, provided $p^2 > 4q$, a positive q and a negative p will give two positive roots. But

$$q = \frac{r_1 r_2(r_3 - r_2)}{(r_2 - r_1)} > 0,$$

and

$$-p = \frac{r_2(r_3 - r_1)}{(r_2 - r_1)} > 0$$

means that $r_3 > r_2 > r_1$ or $r_3 < r_2 < r_1$.

To sum up: If all the r's are positive, de Bray's method of exponential analysis is possible (a) when $D < 6$ and the roots of III are complex; (b) when $D > 6$ and $r_1 > r_2 > r_3$ or when $r_1 < r_2 < r_3$.

Figure 3 gives a picture of the second condition (b) of the preceding paragraph. Suppose an exponential curve is passed through the first *two* points on the empirical curve with ordinates y_0 and y_1. Its equation will be:

$$y = y_0\left(\frac{y_1}{y_0}\right)^{\frac{x}{\delta}} = y_0 r_1^{\frac{x}{\delta}}$$

Suppose also that y_2 is less than the ordinate to this curve when $x = 2\delta$. Now pass an exponential curve through y_1 and y_2 using a new axis of ordinates coinciding with y_1. Its equation is

$$y = y_1\left(\frac{y_2}{y_1}\right)^{\frac{x}{\delta}} = y_1 r_2^{\frac{x}{\delta}},$$

or referred to the original axis:

$$y = y_1 r_2^{\frac{x-\delta}{\delta}}.$$

Now if the graduation is possible without using trigonometric functions, y_3 must be less than the ordinate of this second curve when $x = 3\delta$.

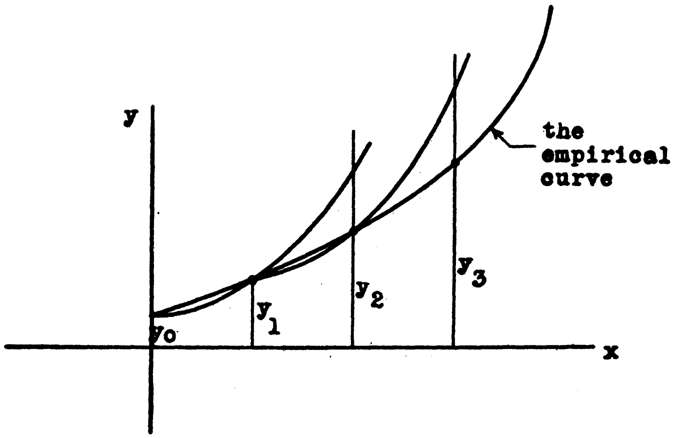

FIG. 3

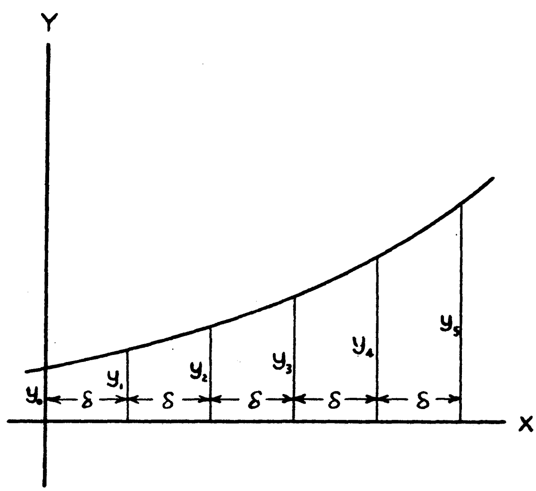

FIG. 4

It is natural to inquire if the state of affairs is not similar to this, for the cases of fitting curves with equations similar to I but having three or four exponential terms on the right hand side instead of only two. If three terms are used (see Fig. 4) to find constants in

(Ia) $$y = A_1 \epsilon^{a_1 x} + A_2 \epsilon^{a_2 x} + A_3 \epsilon^{a_3 x}$$

it is first necessary to find the roots of the cubic

(IIIa)
$$f(x) = \begin{vmatrix} z^3 & z^2 & z & 1 \\ y_5 & y_4 & y_3 & y_2 \\ y_4 & y_3 & y_2 & y_1 \\ y_3 & y_2 & y_1 & y_0 \end{vmatrix}$$

Now, $f(x)$ will have no negative roots if $f(-x)$ has no changes of sign. But writing the conditions that the cofactors of the elements of the first row in the above determinant have the same signs, and assuming that all the y's are positive, one does not get a series of conditions analogous to $r_3 > r_2 > r_1$ or $r_3 < r_2 < r_1$.

In the following, formulas will be derived for finding the constants in equation Ia after the roots of IIIa have been determined. Also formulas will be obtained for finding the constants in

(Ib)
$$y = A_1 \epsilon^{a_1 x} + A_2 \epsilon^{a_2 x} + A_3 \epsilon^{a_3 x} + A_4 \epsilon^{a_4 x}$$

after the roots of

(IIIb)
$$\begin{vmatrix} z^4 & z^3 & z^2 & z & 1 \\ y_7 & y_6 & y_5 & y_4 & y_3 \\ y_6 & y_5 & y_4 & y_3 & y_2 \\ y_5 & y_4 & y_3 & y_2 & y_1 \\ y_4 & y_3 & y_2 & y_1 & y_0 \end{vmatrix} = 0$$

have been found. Both sets of formulas have been tested by an "exponential analysis" of the same body of data, viz., the very accurate recent determinations by the U. S. Bureau of Standards of the saturation pressure of water vapor above 100C.[3]

For the case of three exponential terms in the graduation function, the a's are found by formulas like II or V, after the roots of the cubic are found. If z_1, z_2, z_3 are the roots, the A's are obtained by solving the simultaneous equations

(IVa)
$$\begin{aligned} A_1 + A_2 + A_3 &= y_0 \\ A_1 z_1 + A_2 z_2 + A_3 z_3 &= y_1 \\ A_1 z_1^2 + A_2 z_2^2 + A_3 z_3^2 &= y_2 \end{aligned}$$

[3] Osborne, Stimson, Fiock, and Ginnings: The Pressure of Saturated Water Vapor in the Range 100° to 374°C. Bureau Standards Journal of Research, Vol. 10, Febr. 1933, page 178.

This presents no new difficulty unless two of the roots are conjugate complex numbers. In this event, if we let z_1 = the real positive root, $z_2 = r \cdot \epsilon^{i\theta}$, and $z_3 = r\,\epsilon^{-i\theta}$ the determinant D of the equations IVa may be written

$$D = \begin{vmatrix} 1 & 1 & 1 \\ z_1 & r\epsilon^{i\theta} & r\epsilon^{-i\theta} \\ z_1^2 & r^2\epsilon^{2i\theta} & r^2\epsilon^{-2i\theta} \end{vmatrix}$$

or, expanded in terms of the elements of the first column and their minors,

$$D = 2i[z_1 r^2 \sin 2\theta - (r^3 + z_1^2 r)\sin \theta],$$

a pure imaginary. Similarly,

$$A_1\,D = 2i[r^2 y_1 \sin 2\theta - (y_0 r^3 + y_2 r)\sin \theta],$$

also a pure imaginary, so that A_1 is real. Having calculated A_1, it is substituted in the first two of equations IVa, which are then solved for A_2 and A_3. a_2 and a_3 are then determined by formulas Va and Vb, replacing the subscripts 1 and 2 in those formulas, by the subscripts 2 and 3 respectively. Finally the two exponential terms corresponding to the complex roots of the cubic are combined into a single trigonometric term as in equation VI.

The necessary formulas for the case of four exponential terms in the graduation function will be discussed briefly. The equations

$$\text{(IVb)}\qquad \begin{aligned} A_1 + A_2 + A_3 + A_4 &= y_0 \\ A_1 z_1 + A_2 z_2 + A_3 z_3 + A_4 z_4 &= y_1 \\ A_1 z_1^2 + A_2 z_2^2 + A_3 z_3^2 + A_4 z_4^2 &= y_2 \\ A_1 z_1^3 + A_2 z_2^3 + A_3 z_3^3 + A_4 z_4^3 &= y_3 \end{aligned}$$

have to be solved for the A's. The z's are the roots of IIIb. Two cases will be considered: First case: z_1 and z_2 are complex conjugates and z_3 and z_4 are complex conjugates. Second case: z_1 and z_2 are complex conjugates and z_3 and z_4 are real and positive. In either event A_1 and A_2 are complex conjugates, as will be proved below. Formulas for A_1 are given for both cases. Then A_2 is known since it is the conjugate of A_1. Having found A_1 and A_2, let

$$c_0 = y_0 - (A_1 + A_2)$$

$$c_1 = y_1 - (A_1 z_1 + A_2 z_2)$$

Both c_0 and c_1 are then real. To get A_3 and A_4 solve the equations:

$$\begin{aligned} A_3 + A_4 &= c_0 \\ A_3 z_3 + A_4 z_4 &= c_1 \end{aligned}$$

A pair of exponential terms with conjugate complex coefficients will then be expressed as a single real trigonometric term as in VI.

The determinant of equations IVb may be written

(VII) $$D = (z_1 - z_2)(z_1 - z_3)(z_1 - z_4)(z_2 - z_3)(z_2 - z_4)(z_3 - z_4).$$

First case: Let $z_1 = a + \iota b$, $z_2 = a - \iota b$, $z_3 = \alpha + \iota\beta$, $z_4 = \alpha - \iota\beta$. Then D may be written

(VIIa) $$D = -4\beta b[(a - \alpha)^2 + (b - \beta)^2]\,[(a - \alpha)^2 + (b + \beta)^2],$$

which is real. Now

$$A_1D + A_2D = \begin{vmatrix} y_0 & 1 & 1 & 1 \\ y_1 & z_2 & z_3 & z_4 \\ y_2 & z_2^2 & z_3^2 & z_4^2 \\ y_3 & z_2^3 & z_3^3 & z_4^3 \end{vmatrix} + \begin{vmatrix} 1 & y_0 & 1 & 1 \\ z_1 & y_1 & z_3 & z_4 \\ z_1^2 & y_2 & z_3^2 & z_4^2 \\ z_1^3 & y_3 & z_3^3 & z_4^3 \end{vmatrix}$$

$$= (z_1 - z_2)\begin{vmatrix} 0 & y_0 & 1 & 1 \\ 1 & y_1 & z_3 & z_4 \\ (z_1 + z_2) & y_2 & z_3^2 & z_4^2 \\ (z_1^2 + z_1z_2 + z_2^2) & y_3 & z_3^3 & z_4^3 \end{vmatrix}$$

and this is real since $(z_1 - z_2)$ is a pure imaginary and the minors of the real elements of the first column of the determinant are all pure imaginaries. Hence A_1 and A_2 are complex conjugates since when each is expressed as a quotient of two determinants by Cramer's rule, the sum of the two numerators is real and the common denominator is also real.

For purposes of numerical calculation A_1 may be obtained from

$$A_1 = \frac{NP}{D}$$

in which D is obtained from VIIa,

$$N = y_3 - (z_2 + z_3 + z_4)y_2 + (z_2z_3 + z_2z_4 + z_3z_4)y_1 - (z_2z_3z_4)y_0,$$

$$\text{and } P = (z_2 - z_3)(z_2 - z_4)(z_3 - z_4)$$

$$= 2\beta[(\alpha - a)2b + \iota\{(\alpha - a)^2 + (\beta^2 - b^2)\}], \text{ a complex number.}$$

If $z_1z_2 = r^2$ and $z_3z_4 = \rho^2$, the symmetric functions of the z's in the above formula may be calculated from

$$z_2z_3z_4 = (a - \iota b)\rho^2$$

$$z_2z_3 + z_2z_4 + z_3z_4 = \rho^2 + 2\alpha(a - \iota b)$$

$$z_2 + z_3 + z_4 = (a - \iota b) + 2\alpha$$

For the second case, which is exemplified by the vapor pressure data,

$$\text{(VIIb)} \qquad D = 2\iota b[(a - z_3)^2 + b^2]\,[(a - z_4)^2 + b^2]\,[z_3 - z_4],$$

a pure imaginary. The sum of the two numerators of A_1 and A_2, namely

$$(z_1 - z_2)\begin{vmatrix} 0 & y_0 & 1 & 1 \\ 1 & y_1 & z_3 & z_4 \\ z_1 + z_2 & y_2 & z_3^2 & z_4^2 \\ z_1^2 + z_1 z_2 + z_2^2 & y_3 & z_3^3 & z_4^3 \end{vmatrix}$$

is a pure imaginary, since $(z_1 - z_2)$ has this character, and the determinant has nothing but real elements. Hence A_1 and A_2 are still complex conjugates when z_3 and z_4 are real, z_1 and z_2 being complex conjugates.

For purposes of numerical calculation A_1 may be obtained from

$$A_1 = \frac{N}{(z_1 - z_2)\,(z_1 - z_3)\,(z_1 - z_4)}.$$

Here $(z_1 - z_2)$ is a pure imaginary and the other three factors are complex.

Let

$$N = r_1(\cos\theta_1 + \iota \sin\theta_1)$$

$$z_1 - z_3 = r_2(\cos\theta_2 + \iota \sin\theta_2)$$

$$z_1 - z_4 = r_3(\cos\theta_3 + \iota \sin\theta_3)$$

Then

$$A_1 = \frac{r_1\,[\cos(\theta_1 - \theta_2 - \theta_3) + \iota \sin(\theta_1 - \theta_2 - \theta_3)]}{(z_1 - z_2)\, r_2\, r_3}$$

In calculating N by the formula given for it in the preceding paragraph, the symmetric functions of the z's were obtained from

$$z_2 z_3 z_4 = (a - \iota b) z_3 z_4$$

$$z_2 z_3 + z_2 z_4 + z_3 z_4 = (a - \iota b)(z_3 + z_4) + z_3 z_4$$

$$z_2 + z_3 + z_4 = (a - \iota b) + z_3 + z_4.$$

Example

The first two of the following tables are abstracted from Table 2, p. 178 of Bureau Standards Research Paper No. 523. The third table is abstracted from Table 3, p. 179 et. seq. of that publication. x is the number of degrees centigrade *above* 100°. y is the pressure of saturated water vapor in International Standard Atmospheres. In the first two of the following tables, the values of y are observed values. In the third, they are interpolated or graduated values calculated at the Bureau of Standards.

TABLE I

x	y
0	1.0000
90	12.3887
180	63.3558
270	207.771

TABLE II

x	y
0	1.0000
50	4.6969
100	15.3472
150	39.2566
200	84.7969
250	163.205

TABLE III

x	y
0	1.0000
39	3.4666
78	9.4490
117	21.612
156	43.392
195	78.974
234	133.64
273	215.37

The observed values of y in Table I are reproduced by the following formula used in conjunction with a standard six place table of logarithms and trigonometric functions:

$$y = 3.967433\, \epsilon^{.01539540x} \cos(.4085758x - 75^\circ 24' 03''.7). \tag{I}$$

The observed values of y in Table II are reproduced by the following formula used in conjunction with a standard six place table of logarithms and trigonometric functions.

$$\begin{aligned} y &= 3.0253744\, \epsilon^{.01515605x} \\ &+ 2.2171657\, \epsilon^{.011500716x} \cos(155^\circ 59' 35''.5 - 0.7899232x). \end{aligned} \tag{II}$$

Hence the formula is presumably an excellent one for interpolation between the values of y listed in Table II, if the greatest accuracy is not needed.[4]

The values of y in Table III are reproduced exactly to five significant figures by the following formula used in conjunction with a standard six place table of logarithms and trigonometric functions.

$$y = 3.8902543\, \epsilon^{.01413920x} - .164787\, \epsilon^{-.0216930x}$$

$$+ 2.743000\, \epsilon^{.009884290x} \cos(.7860725x + 186°28'53''.2).$$

By means of this formula the saturation pressure of water vapor was calculated for every five degrees from 100°C to 370°C in order to make comparisons with the corresponding "smoothed" values in Table 2 of the Bureau of Standards publication referred to above. The discrepancies were never more than one in the fourth significant figure and generally less. The poorest agreement was in the ranges of temperature from 100°C to 135°C and from 245°C to 270°C.

It is a pleasure to acknowledge the intelligent and painstaking assistance of Mr. G. D. Lambert, undergraduate student at Washington University, for doing most of the computing.

WASHINGTON UNIVERSITY,
ST. LOUIS, MO.

---

[4] The values of y in Table III (not counting the value of y for $x = 0$) are reproduced by it with an average error of .13% and a largest error (for $x = 234°$) of .30%. Four of the errors are negative and three positive.