# THE FUNCTION INVERFC θ

By J. R. PHILIP*

[*Manuscript received November* 11, 1959]

*Summary*

The function inverfc θ arises in certain diffusion problems when concentration is taken as an independent variable. It enters into a general method of exact solution of the concentration-dependent diffusion equation. An account is given of the properties of this function, and of its derivatives and integrals. The function

$$B(\theta)=(2/\pi^{\frac{1}{2}})\exp[-(\text{inverfc }\theta)^2]$$

is intimately connected with the first integral of inverfc θ and with its derivatives. Tables of inverfc θ and $B(\theta)$ are given.

## I. INTRODUCTION

The solution of one-dimensional diffusion problems is usually sought in the form

concentration=explicit function of distance and time.

It has become increasingly evident, however, that there are occasions when it is simpler, and more illuminating, to seek the solution in the form

distance=explicit function of concentration and time.

In particular, the latter approach has proved fruitful when applied to concentration-dependent diffusion (Philip 1955) and when applied to problems where concentration-dependent diffusion is combined with a first-order (not necessarily linear) phenomenon (Philip 1957).

In these connexions, it was found convenient (Philip 1955) to introduce the notation " inverfc " to denote the inverse of the function

$$\text{erfc }x=\frac{2}{\pi^{\frac{1}{2}}}\int_x^\infty \exp(-\zeta^2)\mathrm{d}\zeta. \qquad \text{(1.1)}$$

Until now there has been no urgent need to examine in detail the properties of the inverfc function. However, inverfc θ and its first derivative and first integral with respect to θ enter intimately into the recently found general method of exact solution of the concentration-dependent diffusion equation (Philip 1960). This account of the properties of inverfc θ, its derivatives, and its integrals, therefore forms an essential supplement to Philip (1960). The tabulations of the functions inverfc θ and $B(\theta)$ given here will frequently be needed when the method of Philip (1960) is applied.

* Division of Plant Industry, C.S.I.R.O., Canberra.

The concept of inverfc as the inverse of erfc leads to definition of the function through (**1.2**):

$$\theta = \text{erfc } (\text{inverfc } \theta). \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{1.2})$$

An alternative *de novo* definition of inverfc follows from equations (**3.4**) and (**4.1**) of Philip (1960). In this way the function may be introduced as the solution, $F = \text{inverfc } \theta$, of the equation

$$\frac{dF}{d\theta}\int_0^\theta F d\theta = -\tfrac{1}{2}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{1.3})$$

subject to the conditions

$$F(1)=0\ ; \quad 0 \leqslant \theta \leqslant 1, \ F \geqslant 0. \quad \ldots\ldots\ldots\ldots \quad (\mathbf{1.4})$$

The following elementary results come directly from the known properties of erfc:

$$\text{inverfc } 0 = +\infty\ ; \quad \text{inverfc } 1 = 0\ ; \quad \text{inverfc } 2 = -\infty, \quad \ldots \quad (\mathbf{1.5})$$

$$\text{inverfc } (2-\theta) = -\text{inverfc } \theta. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{1.6})$$

We shall deal almost exclusively with the interval in $\theta$, $0 \leqslant \theta \leqslant 1$; it is a trivial matter to extend the results to the whole interval $0 \leqslant \theta \leqslant 2$ by means of (**1.6**). Note that inverfc $\theta$ is defined only within the latter interval.

TABLE 1
inverfc $\theta$ COMPUTED FROM SERIES (**2.4**)

| $\theta$ | inverfc $\theta$ Computed from Series (**2.4**) | | | inverfc $\theta$ Exact Value |
|---|---|---|---|---|
| | Three Terms | Four Terms | Five Terms | |
| 0·6 | 0·3706458 | 0·3707451 | 0·3707570 | 0·3708072 |
| 0·7 | 0·2724424 | 0·2724557 | 0·2724566 | 0·2724627 |
| 0·8 | 0·1791423 | 0·1791431 | 0·1791431 | 0·1791434 |
| 0·9 | 0·0888560 | 0·0888560 | 0·0888560 | 0·0888560 |

## II. POWER SERIES FOR inverfc $\theta$

We introduce the power series connected with erfc:

$$\tfrac{1}{2}\pi^{\frac{1}{2}}(1-\text{erfc } x) = x - \frac{x^3}{3} + \frac{x^5}{2!5} - \frac{x^7}{3!7} + \frac{x^9}{4!9} - \ldots \quad (\mathbf{2.1})$$

Putting

$$\vartheta = \tfrac{1}{2}\pi^{\frac{1}{2}}(1-\theta), \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{2.2})$$

and writing $x$ for inverfc $\theta$, we have

$$\vartheta = x - \frac{x^3}{3} + \frac{x^5}{2!5} - \frac{x^7}{3!7} + \frac{x^9}{4!9} - \ldots \quad \ldots\ldots\ldots \quad (\mathbf{2.3})$$

Suppose now, that inverfc θ (i.e. $x$) may be expanded as a power series in $\vartheta$. Then we may formally establish this series by equating coefficients of powers of $\vartheta$ on each side of (**2.3**). The result is

$$\text{inverfc}\,\theta=\vartheta+\tfrac{1}{3}\vartheta^3+\frac{7}{30}\vartheta^5+\frac{127}{630}\vartheta^7+\frac{4369}{22680}\vartheta^9+\ldots \quad \ldots \quad (\mathbf{2.4})$$

No simple general expression for the coefficients is apparent. It will be shown later in Section IV that (**2.4**) may be derived directly from the Taylor expansion of inverfc θ about θ=1. The series of (**2.3**) is uniformly convergent. Presumably the series of (**2.4**) converges for $|\vartheta|<\tfrac{1}{2}\pi^{\frac{1}{2}}$. It provides a useful means of calculating inverfc θ in the neighbourhood of θ=1. Table 1 gives a comparison of the exact value of inverfc θ with that computed from the first few terms of series (**2.4**).

## III. Asymptotic Forms of inverfc θ, θ Small

For large values of $x$ (=inverfc θ), we have the well-known asymptotic result:

$$\theta\approx\frac{\exp(-x^2)}{\pi^{\frac{1}{2}}x}. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{3.1})$$

(**3.1**) is equivalent to

$$x^2\approx-\log\theta-\tfrac{1}{2}\log\pi x^2,$$

which has the continued logarithmic form

$$x^2\approx-\log\theta-\tfrac{1}{2}\log[\pi(-\log\theta-\tfrac{1}{2}\log[\ldots$$

Accordingly we have the approximation for θ small:

$$\text{inverfc}\,\theta=\{-\log\theta-\tfrac{1}{2}\log[\pi(-\log\theta-\tfrac{1}{2}\log[\ldots\}^{\frac{1}{2}}. \quad \ldots \quad (\mathbf{3.2})$$

As far as the author knows, no formal study has been made of the convergence of continued logarithms. The convergence of (**3.2**) is rapid for θ small. See Table 2. In this table the symbol $S_n$ denotes the $n$th member of the sequence formed by terminating the repeated logarithm at successive log θ's. Thus,

$$S_1=(-\log\theta)^{\frac{1}{2}};$$
$$S_2=(-\log\theta-\tfrac{1}{2}\log[\pi(-\log\theta)])^{\frac{1}{2}};$$
$$S_3=(-\log\theta-\tfrac{1}{2}\log[\pi(-\log\theta-\tfrac{1}{2}\log\{\pi(-\log\theta)\})])^{\frac{1}{2}};$$

and so on.

It is evident that the limit to the accuracy of using (**3.2**) for θ small is set by the limited accuracy of (**3.1**) rather than by the rate of convergence of the sequence $S_n$. Note that $S_2$ proves a better approximation to inverfc θ than do the higher members of the sequence.

TABLE 2
inverfc θ COMPUTED FROM (**3.2**)

| $\theta$ | $S_1$ | $S_2$ | $S_3$ | $S_4$ | inverfc θ Exact Value |
|---|---|---|---|---|---|
| $10^{-6}$ | 3·7169 | 3·4540 | 3·4646 | 3·4642 | 3·4589 |
| $10^{-4}$ | 3·0349 | 2·7437 | 2·7620 | 2·7608 | 2·7509 |
| $10^{-2}$ | 2·1460 | 1·8081 | 1·8549 | 1·8480 | 1·8214 |

Pollack (1956) has established an inequality which leads to the following improved approximation

$$\theta \approx \frac{2 \exp(-x^2)}{\pi^{\frac{1}{2}}\{x+\sqrt{(x^2+4/\pi)}\}}. \qquad \textbf{(3.3)}$$

This yields the better approximation

$$\text{inverfc}\ \theta = \{-\log\theta - \sinh^{-1}\sqrt{\tfrac{1}{4}\pi(-\log\theta - \sinh^{-1}\sqrt{[\tfrac{1}{4}\pi(-\log\theta\ .\ .\ .}}\}^{\frac{1}{2}}. \qquad \textbf{(3.4)}$$

(**3.4**) is more accurate than (**3.2**), and converges at about the same rate; but it involves $\sinh^{-1}$, which is scarcely any simpler than inverfc.

The following result follows from (**3.2**) or (**3.3**)

$$\lim_{\theta\to 0} \frac{\text{inverfc}\ \theta}{(-\log\theta)^{\frac{1}{2}}} = 1.$$

## IV. THE DERIVATIVES AND INTEGRALS OF inverfc θ

Differentiating equation (**1.2**), we obtain

$$\frac{d}{d\theta}(\text{inverfc}\ \theta) = -\tfrac{1}{2}\pi^{\frac{1}{2}} \exp[(\text{inverfc}\ \theta)^2]. \qquad \textbf{(4.1)}$$

It is convenient to introduce the function

$$B(\theta) = \frac{2}{\pi^{\frac{1}{2}}} \exp[-(\text{inverfc}\ \theta)^2]. \qquad \textbf{(4.2)}$$

We then have

$$\frac{d}{d\theta}(\text{inverfc}\ \theta) = -\frac{1}{B}. \qquad \textbf{(4.3)}$$

In addition,

$$\frac{dB}{d\theta} = 2\ \text{inverfc}\ \theta, \qquad \textbf{(4.4)}$$

and, in general ($m\neq 0$, $n\neq 0$),

$$\frac{d}{d\theta}\left[\frac{(\text{inverfc}\ \theta)^m}{B^n}\right] = -\frac{1}{B^{n+1}}[2n(\text{inverfc}\ \theta)^{m+1} + m(\text{inverfc}\ \theta)^{m-1}]. \qquad \textbf{(4.5)}$$

This result is useful for generating the higher derivatives* of inverfc θ. We have, for example,

$$\frac{d^2}{d\theta^2}(\text{inverfc }\theta)=\frac{1}{B^2}(2\text{ inverfc }\theta),$$

$$\frac{d^3}{d\theta^3}(\text{inverfc }\theta)=-\frac{1}{B^3}\{8(\text{inverfc }\theta)^2+2\},$$

$$\frac{d^4}{d\theta^4}(\text{inverfc }\theta)=\frac{1}{B^4}\{48(\text{inverfc }\theta)^3+28\text{ inverfc }\theta\},$$

$$\frac{d^5}{d\theta^5}(\text{inverfc }\theta)=-\frac{1}{B^5}\{384(\text{inverfc }\theta)^4+368(\text{inverfc }\theta)^2+28\},$$

$$\frac{d^6}{d\theta^6}(\text{inverfc }\theta)=\frac{1}{B^6}\{3840(\text{inverfc }\theta)^5+5216(\text{inverfc }\theta)^3+1016\text{ inverfc }\theta\},$$

$$\frac{d^7}{d\theta^7}(\text{inverfc }\theta)=-\frac{1}{B^7}\{46{,}080(\text{inverfc }\theta)^6+81{,}792(\text{inverfc }\theta)^4 +27{,}840(\text{inverfc }\theta)^2+1016\}.$$

It is evident that, *for* n *odd*,

$$\frac{d^n}{d\theta^n}(\text{inverfc }\theta)=-\frac{1}{B^n}(a_{n-1}(\text{inverfc }\theta)^{n-1}+a_{n-3}(\text{inverfc }\theta)^{n-3}+\ldots+a_0),$$

and, *for* n *even*,

$$\frac{d^n}{d\theta^n}(\text{inverfc }\theta)=\frac{1}{B^n}\{a_{n-1}(\text{inverfc }\theta)^{n-1}+a_{n-3}(\text{inverfc }\theta)^{n-3} +\ldots+a_1\text{ inverfc }\theta\}.$$

In both cases the coefficients $a_{n-1}$, etc. are all positive.

Now $2/\pi^{\frac{1}{2}}\geqslant B\geqslant 0$ throughout the interval $0\leqslant\theta\leqslant 2$, whilst inverfc θ is positive in $0\leqslant\theta<1$, zero at $\theta=1$, and negative in $1<\theta\leqslant 2$. It therefore follows that, in the interval $0\leqslant\theta<1$,

$\frac{d^n}{d\theta^n}(\text{inverfc }\theta)$ is positive if $n$ is even, negative if $n$ is odd;

at $\theta=1$,

$\frac{d^n}{d\theta^n}(\text{inverfc }\theta)$ is zero if $n$ is even, negative if $n$ is odd;

in the interval $1<\theta\leqslant 2$,

$\frac{d^n}{d\theta^n}(\text{inverfc }\theta)$ is negative whether $n$ is even or odd.

* I am indebted to the referee for remarks which suggest the following, more elegant, treatment of the higher derivatives of inverfc θ.

$F$=inverfc θ satisfies the equation

$$d^2F/d\theta^2=2F(dF/d\theta)^2. \qquad \text{(A)}$$

This may be established by differentiating (**1.3**) with respect to θ. Now, if $P_n(F)$ denotes a polynomial in $F$, and

$$d^nF/d\theta^n=P_n(F)(dF/d\theta)^n, \qquad \text{(B)}$$

it follows by differentiation and use of (**A**) that

$$d^{n+1}F/d\theta^{n+1}=P_{n+1}(F)(dF/d\theta)^{n+1},$$

where

$$P_{n+1}(F)=(2nF+d/dF)P_n(F). \qquad \text{(C)}$$

Now (**B**) is true for $n=1$, and $P_1(F)=1$. Therefore, $P_n(F)$ for all $n>1$ follows at once from (**C**), giving a simple means of determining the higher derivatives of inverfc θ.

We have the particular results :

$$(-1)^n \frac{d^n}{d\theta^n} (\text{inverfc } 0) = \infty,$$

$$\frac{d^n}{d\theta^n} (\text{inverfc } 2) = -\infty.$$

The values of the first nine derivatives of inverfc $\theta$ at $\theta=1$ are

$$-\tfrac{1}{2}\pi^{\frac{1}{2}},\ 0,\ -2(\tfrac{1}{2}\pi^{\frac{1}{2}})^3,\ 0,\ -28(\tfrac{1}{2}\pi^{\frac{1}{2}})^5,\ 0,\ -1016(\tfrac{1}{2}\pi^{\frac{1}{2}})^7,\ 0,\ -69{,}904(\tfrac{1}{2}\pi^{\frac{1}{2}})^9.$$

It follows from these results that equation (**2.4**) may be established by applying Taylor's theorem to the right-hand side of the identity

$$\text{inverfc } \theta = \text{inverfc } [1-(1-\theta)].$$

We also note that it follows from (**4.4**) that

$$\frac{d^n B}{d\theta^n} = 2\frac{d^{n-1}}{d\theta^{n-1}} (\text{inverfc } \theta). \qquad \ldots\ldots\ldots\ldots \quad (4.6)$$

It is readily established by integration by parts, or by use of (**4.1**) in (**1.3**), or by integrating (**4.4**), that

$$\int_0^\theta \text{inverfc } \theta \, d\theta = \frac{1}{\pi^{\frac{1}{2}}} \exp(-\text{inverfc } \theta)^2 = \tfrac{1}{2}B. \qquad \ldots \quad (4.7)$$

A further integration yields

$$\int_0^\theta \int_0^\theta \text{inverfc } \theta \, d\theta d\theta = \frac{1}{\sqrt{(2\pi)}} \text{erfc } (\sqrt{2} \text{ inverfc } \theta).$$

This and the higher integrals of inverfc $\theta$ do not appear to be of significance in the present developments.

## V. The Function $B(\theta)$

We have seen that $B(\theta)$ is simply related to the first derivative, and to the first integral, of inverfc $\theta$. For this reason it proves of primary importance in the development of the general method of exact solution of the concentration-dependent diffusion equation (Philip 1960).

We note from (**1.6**) and (**4.2**) that

$$B(2-\theta) = B(\theta). \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (5.1)$$

We have already remarked on the simple relation between derivatives of inverfc $\theta$ and those of $B$. It follows that the Taylor expansion of $B(\theta)$ about $\theta=1$ yields as the power series for $B$

$$B(\theta) = \frac{2}{\pi^{\frac{1}{2}}}\left[1-\vartheta^2-\frac{\vartheta^4}{6}-\frac{7}{90}\vartheta^6-\frac{127}{2520}\vartheta^8-\frac{4369}{113400}\vartheta^{10}-\ldots\right], \quad \ldots \quad (5.2)$$

where $\vartheta$ is again defined by (**2.2**). Presumably the series of (**5.2**) converges for $|\vartheta| \leqslant \tfrac{1}{2}\pi^{\frac{1}{2}}$. It enables $B$ to be calculated readily in the neighbourhood of $\theta=1$.

The behaviour of $B$ near $\theta=0$ is of interest. Approximation (**3.1**) applied in (**4.2**) yields

$$B(\theta)\approx 2\theta(-\log\theta)^{\frac{1}{2}}, \qquad \ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{5.3})$$

and it may be shown that

$$\lim_{\theta\to 0}\frac{B(\theta)}{2\theta\,(-\log\theta)^{\frac{1}{2}}}=1.$$

It follows that, as $\theta\to 0$, $B\to 0$ more rapidly* than does $\theta^{1-\varepsilon}$, where $\varepsilon$ is any non-zero positive quantity, and more slowly than does $\theta$.

## VI. Tables of inverfc $\theta$ and $B(\theta)$

The only existing table of inverfc $\theta$ known to the author is in Fowle (1921, p. 60). The column of the table headed $v/c$ gives $\theta$ in the present notation, and that headed $2q$ gives values of 2 inverfc $\theta$ to four or five significant figures. In connexion with Philip (1960) it is helpful to have a table of inverfc $\theta$ readily available. In the course of constructing the table of $B(\theta)$, it was a simple matter

Table 3

The functions inverfc $\theta$ and $B(\theta)$

| $\theta$ | inverfc $\theta$ | $B(\theta)$ | $\theta$ | inverfc $\theta$ | $B(\theta)$ |
|---|---|---|---|---|---|
| 0 | $\infty$ | 0 | 0·40 | 0·595 116 1 | 0·791 851 9 |
| $10^{-6}$ | 3·458 911 | 0·000 007 177 8 | 0·45 | 0·534 159 1 | 0·848 280 6 |
| $10^{-5}$ | 3·122 587 | 0·000 065 742 | 0·50 | 0·476 936 3 | 0·898 807 9 |
| $10^{-4}$ | 2·750 936 | 0·000 583 27 | 0·55 | 0·422 680 2 | 0·943 766 6 |
| $10^{-3}$ | 2·326 754 | 0·005 026 6 | 0·60 | 0·370 807 2 | 0·983 423 2 |
| $10^{-2}$ | 1·821 386 | 0·040 898 3 | 0·65 | 0·320 858 3 | 1·017 992 1 |
| 0·05 | 1·385 904 | 0·165 219 5 | 0·70 | 0·272 462 7 | 1·047 646 6 |
| 0·10 | 1·163 087 | 0·291 711 6 | 0·75 | 0·225 312 1 | 1·072 526 1 |
| 0·15 | 1·017 902 | 0·400 379 2 | 0·80 | 0·179 143 4 | 1·092 741 7 |
| 0·20 | 0·906 193 8 | 0·496 384 2 | 0·85 | 0·133 726 9 | 1·108 379 8 |
| 0·25 | 0·813 419 8 | 0·582 241 7 | 0·90 | 0·088 856 0 | 1·119 505 3 |
| 0·30 | 0·732 869 1 | 0·659 472 6 | 0·95 | 0·044 341 3 | 1·126 162 8 |
| 0·35 | 0·660 854 4 | 0·729 098 6 | 1·00 | 0 | 1·128 379 2 |

to develop a new and more accurate table of inverfc $\theta$. Details are given below, and the resulting tabulation is presented in Table 3. No graph of inverfc $\theta$ is given, since the shape of erfc $x$ is well known.

No table of $B(\theta)$ is known to the author. The tabulation of this function, which is also given in Table 3, was constructed with the aid of National Bureau of Standards (1954) tables by methods described below. Figure 1 gives the plot of $B(\theta)$.

*Table of inverfc* $\theta$. The table of inverfc $\theta$ was constructed from the National Bureau of Standards (1954) tables of erf $x$ by a process of inverse interpolation.

* Suppose $\lim_{\theta\to\theta_0} P(\theta)=0$; $\lim_{\theta\to\theta_0} Q(\theta)=0$. Then we say that, as $\theta\to\theta_0$, $P\to 0$ more rapidly than does $Q$, provided that $\lim_{\theta\to\theta_0}\frac{P}{Q}(\theta)=0$.

" Linear " interpolation of the type suggested in the introduction to those tables proved sufficiently accurate to ensure that errors in the final place given would not exceed unity. Twenty comparisons with Fowle's table were possible; in every case the final place of Fowle's tabulation of $2q$ (i.e. 2 inverfc θ) was confirmed.

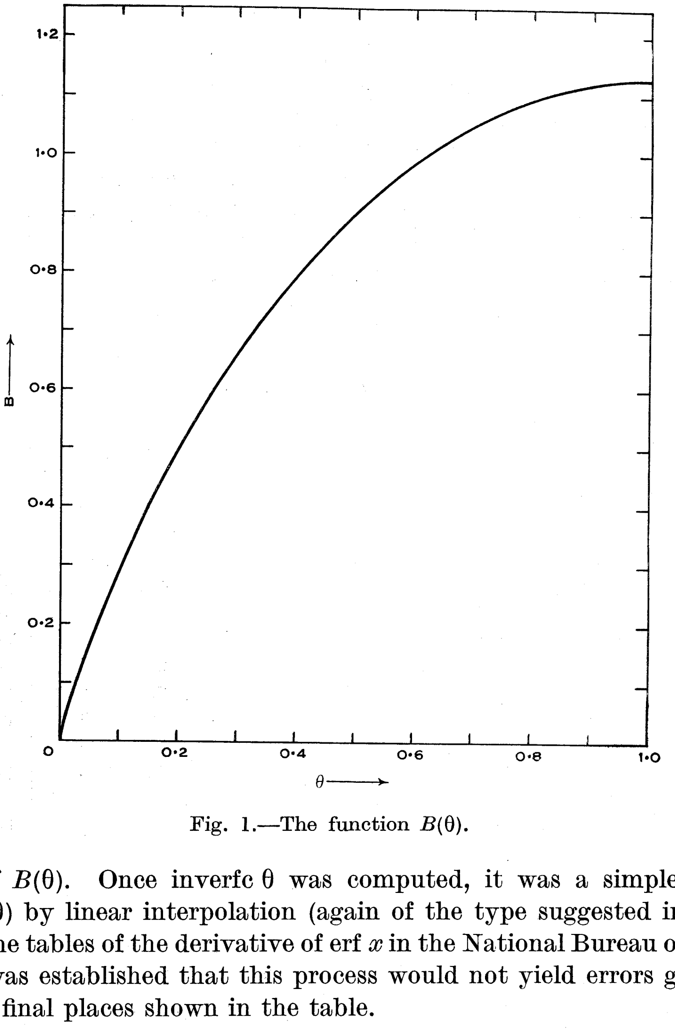


Fig. 1.—The function $B(\theta)$.

*Table of* $B(\theta)$. Once inverfc θ was computed, it was a simple matter to calculate $B(\theta)$ by linear interpolation (again of the type suggested in the introduction) in the tables of the derivative of erf $x$ in the National Bureau of Standards tables. It was established that this process would not yield errors greater than unity in the final places shown in the table.

Most of each table was checked by differencing.

## VII. References

Fowle, F. E. (1921).—" Smithsonian Physical Tables." 7th Ed. (Smithsonian Institution: Washington.)

National Bureau of Standards (1954).—" Tables of the Error Function and its Derivative." Applied Maths. Series 41. (U.S. Govt. Printing Office: Washington.)

Philip, J. R. (1955).—*Trans. Faraday Soc.* **51**: 885.

Philip, J. R. (1957).—*Aust. J. Phys.* **10**: 29.

Philip, J. R. (1960).—*Aust. J. Phys.* **13**: 1.

Pollack, H. O. (1956).—*Rep. Statist. Appl. Res. Un. Jap. Sci. Engrs.* **4**: 40.