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Comment on "Analytical series expressions for Hantush's *M* and *S* functions" by Michael G. Trefry

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Trefry [1998] has presented an interesting study of properties of the integral

$$M(\alpha, \beta) = \frac{2}{\pi}\int_0^\alpha \frac{\exp[-\beta(1+y^2)]}{1+y^2}\,dy, \tag{1}$$

a function that arises in analytical solutions to various groundwater flow problems, including mounding [e.g., *Hantush*, 1965, 1967]. *Trefry* [1998, p. 909], in reference to computation of (1), states

> The advent of advanced mathematical tools, for example, the computer package *Mathematica* [*Wolfram*, 1992] and others like it, has made such numerical evaluations easy. However, theoretical studies of percolation may be hampered by using numerical quadratures to evaluate the mounding integrals, as valuable functional relationships involving the arguments α and β can be obscured in the numerics. For this reason it is preferable to pursue analytical solution of these important integrals.

We endorse these statements, with the proviso that such expressions should be analytically transparent, and not unduly complicated, if they are to permit widespread practical utility. For example, series with large numbers of terms are likely not very useful in this context. Thus an expression like (23) of *Trefry* [1998] (restated below; see equation (3)), which has only a few terms, would be extremely useful if accurate enough for the recommended range of α and β ($\leq\frac{1}{2}$ and $\leq\frac{3}{2}$, respectively).

Trefry [1998] showed that exact analytical formulas for evaluating (1) are available in the form of infinite series. One focus of Trefry's study was on the convergence of different forms of these series, as alternatives to quadrature for finding numerical values of *M*. *Trefry* [1998] concluded that the most rapidly convergent, and thus preferable, series for this purpose is

$$M_{T,\infty} = \frac{2}{\pi}\left\{\arctan(\alpha) - \alpha\exp(-\beta)\sum_{n=0}^{\infty}\left[\frac{\beta^n}{n!}\sum_{k=0}^{n-1}\frac{(-\alpha^2)^k}{2k+1}\right]\right\}. \tag{2}$$

However, with respect to (2), as pointed out by *Trefry* [1998, p. 911], "large values of α or β may mitigate against rapid convergence." He suggests (p. 912) that (2) "is most useful for the domain $\alpha^2\beta < 1$." For example, the two-term, truncated expansion of (2),

$$M_{T,2} = \frac{2}{\pi}\left[\arctan(\alpha) - \alpha\beta\exp(-\beta)\left(1 + \frac{\beta}{2} - \frac{\alpha^2\beta}{6}\right)\right], \tag{3}$$

was suggested as a useful approximation with accuracy of "5% for $\alpha \leq \frac{1}{2}$ and $\beta \leq \frac{3}{2}$" [*Trefry*, 1998, p. 912]. Our purpose in this comment is to suggest, for this range, (1) an alternative series to equation (2) for computation of *M* and (2) a simple approximation that improves on equation (3).

In (1) we expand the denominator as a power series for $y < 1$ (i.e., $\alpha < 1$). Then, term-by-term integration is possible. The complete series is given by

$$M_{1,\infty} = \frac{\exp(-\beta)}{\sqrt{\pi\beta}}\sum_{n=0}^{\infty}(-1)^n(2n-1)!! \cdot\left[\frac{\operatorname{erf}(\alpha\sqrt{\beta})}{(2\beta)^n} - \frac{\alpha\exp(-\alpha^2\beta)}{\sqrt{\pi\beta}} \cdot\sum_{k=0}^{n-1}\frac{\alpha^{2(n-1-k)}}{(2n-1-2k)!!(2\beta)^k}\right]. \tag{4}$$

Equation (4) can be written as

$$M_{1,0}f(\alpha, \beta) = \frac{\exp(-\beta)\operatorname{erf}(\alpha\sqrt{\beta})}{\sqrt{\pi\beta}}f(\alpha, \beta),$$

where the fraction is the first term in the expansion and f represents the rest of the series. We derive an approximation for (4) by choosing a simple form for f. Thus we approximate f by taking the limiting case of $\beta = 0$, which gives $f(\alpha, \beta) \approx f(\alpha, 0) = \arctan(\alpha)/\alpha$, so that we obtain an exact result in this limit. We choose this limit since an examination of (4) shows clearly that computational difficulties are likely for small β.

Note that (4) represents the asymptotic series of (1) as $\beta \to \infty$, valid for $\alpha < 1$. Hence it will converge very rapidly for large β. Further, observe that it is an alternating series and would thus, a priori, be expected to be relatively poor for predicting *M* if large numbers of terms were used. In addition, numerical difficulties could arise if large numbers of terms are used. Convergence would undoubtedly be improved if it was resumed as a nonalternating series. Rather than proceed down this obvious path, we shall use the above estimate of f together with the first term in the expansion to estimate *M*, this approximation having the virtue of being very simple.

In Table 1 we compare (3) (the expression suggested by

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Table 1. Comparison of $M_{T,2}$ (From Equation (3)), $M_{1,0}f(\alpha,\ 0)$, and $M_{1,2}$ (From Equation (4)) for Various Cases of $\alpha \leq \frac{1}{2}$ and $\beta \leq \frac{3}{2}$

		$M_{T,2}$ [*Trefry*, 1998]		$M_{1,0}f(\alpha,\ 0)$		$M_{1,2}$	
α	β	R*	A†	R	A	R	A
1/4	1/4	−0.279	0.0337	0.00839	−0.00101	−0.00337	0.000407
	1/2	−2.40	0.224	0.0168	−0.00157	−0.00335	0.000313
	3/4	−8.71	0.632	0.0251	−0.00182	−0.00332	0.000241
	1	−22.3	1.25	0.0334	−0.00188	−0.00330	0.000186
	5/4	−47.1	2.05	0.0417	−0.00182	−0.00328	0.000143
	3/2	−88.3	2.98	0.0500	−0.00169	−0.00325	0.000110
1/2	1/4	−0.284	0.0639	0.122	−0.0276	−0.196	0.0442
	1/2	−2.47	0.425	0.243	−0.0419	−0.191	0.0328
	3/4	−9.10	1.20	0.362	−0.0477	−0.185	0.0244
	1	−23.6	2.37	0.479	−0.0482	−0.180	0.0181
	5/4	−50.5	3.89	0.595	−0.0459	−0.175	0.0134
	3/2	−95.9	5.65	0.709	−0.0417	−0.169	0.0100

In each case, we show both the relative (1 − (approximation/exact value)) and absolute errors (approximation − exact value), as percentages.

*R is relative error.

†A is absolute error.

Trefry [1998]) and, as discussed above, $M_{1,0}f(\alpha,\ 0)$. The values of α and β considered are those given by *Trefry* [1998] as the range over which (3) is useful. Both relative and absolute errors are given in the table. For $\alpha = \frac{1}{2}$ and $\beta = \frac{3}{2}$, the absolute error of Trefry's approximation is 5.65%. For $\alpha = \beta = \frac{1}{2}$, the relative error is <2.5%. From Table 1 we observe that (3) is a very poor estimator of M, even in the recommended parameter range $\alpha \leq \frac{1}{2}$, $\beta \leq \frac{3}{2}$. Obviously, improved estimates could be obtained if further terms were retained in (2) [*Trefry*, 1998]. However, in that case, the elegant simplicity of the analytical formula would be lost. In order to compare the series (2) with the series (4), we took the same number of terms as did *Trefry* [1998] to derive (3). This expansion, $M_{1,2}$, performs very well for the cases considered in Table 1. In contrast to the other cases and as noted above, the accuracy of the estimates improves with increasing β, this behavior being, of course, in keeping with (4) being an asymptotic expansion for β. $M_{1,2}$ is, however, a slightly more complicated expression than either of the other two cases, a characteristic that is consistent with its increased accuracy. $M_{1,0}f(\alpha,\ 0)$ is simpler than $M_{1,2}$, but it is also a very accurate estimator of M, with a maximum relative error of <0.71% in the parameter range used.

In summary, we have presented an alternative series for estimating M to those investigated by *Trefry* [1998]. This alternative is superior to (2) if only a couple of terms are used, as shown in Table 1. Its accuracy improves with increasing β. In the case of the one-term expansion, $M_{1,0}f(\alpha,\ 0)$, we have presented a compact alternative to (3), the expression recommended by *Trefry* [1998]. For instance, in the case of $\alpha = \frac{1}{2}$, $\beta = \frac{3}{2}$, the given bounds for use of (3) [*Trefry*, 1998], we find that his maximum relative error is 95.9% (the relative error is much more acceptable if the range of β is restricted to $\frac{1}{2}$, in which case the maximum relative error is 2.47%), whereas the more simple (5) is only 0.709% in error.

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